



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 09:50 AM UTC

PDB ID : 1I4V / pdb_00001i4v
Title : SOLUTION STRUCTURE OF THE UMUD' HOMODIMER
Authors : Ferentz, A.E.; Walker, G.C.; Wagner, G.
Deposited on : 2001-02-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

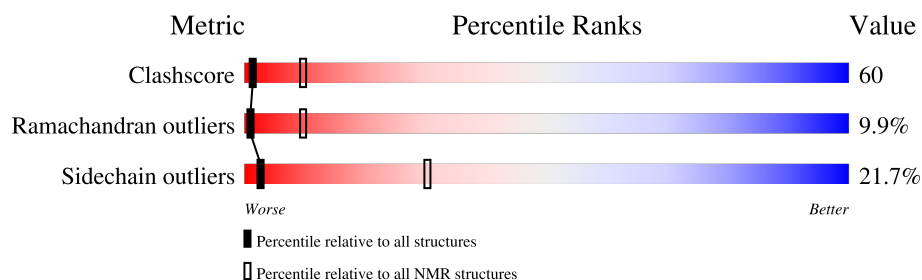
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	115	
1	B	115	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:38-A:139, B:38-B:139 (204)	1.37	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 8, 9, 10, 17
2	1, 12, 14, 18
3	3, 15, 19
4	13, 16
Single-model clusters	7; 11; 20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3474 atoms, of which 1744 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UMUD' PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1737	550	872	141	171	3	
1	B	115	Total	C	H	N	O	S	0
			1737	550	872	141	171	3	

There are 2 discrepancies between the modelled and reference sequences:

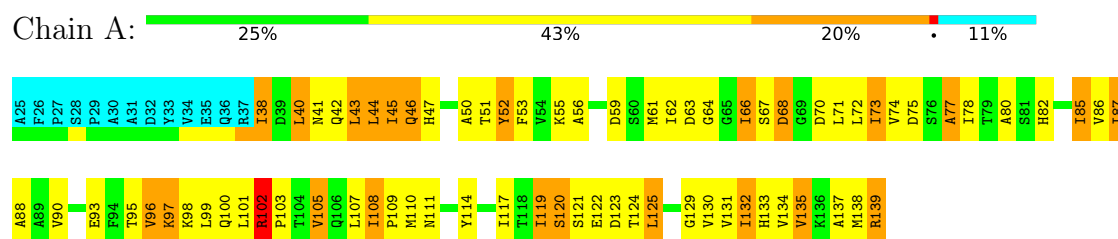
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	GLY	engineered mutation	UNP P04153
B	25	ALA	GLY	engineered mutation	UNP P04153

4 Residue-property plots

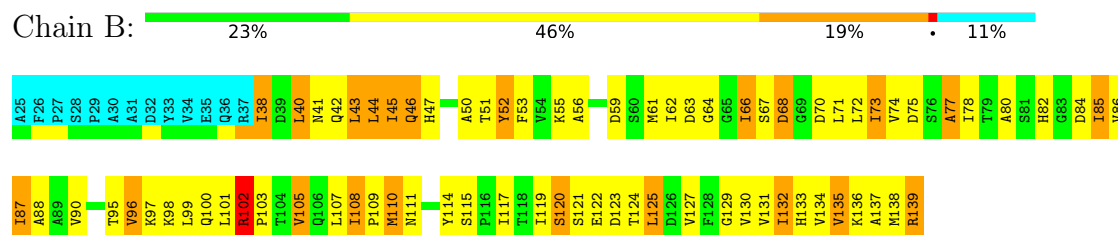
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: UMUD' PROTEIN



• Molecule 1: UMUD' PROTEIN

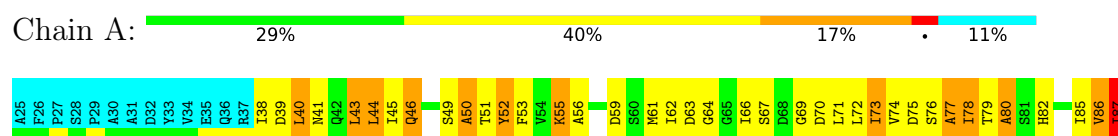


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

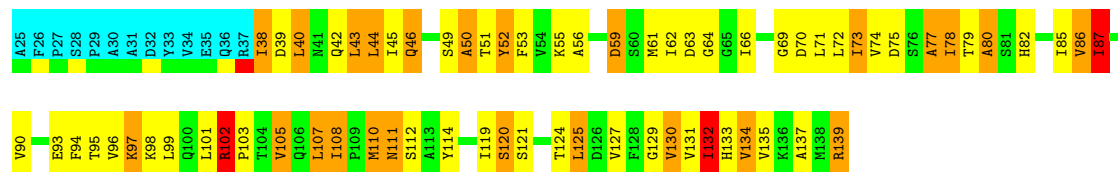
4.2.1 Score per residue for model 1

• Molecule 1: UMUD' PROTEIN



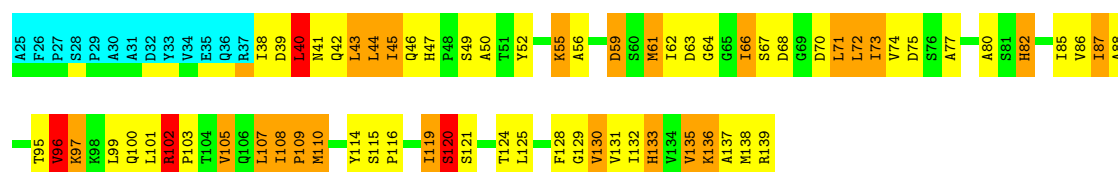


• Molecule 1: UMUD' PROTEIN

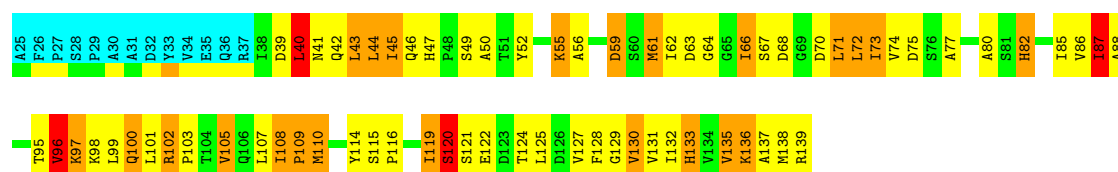


4.2.2 Score per residue for model 2

• Molecule 1: UMUD' PROTEIN

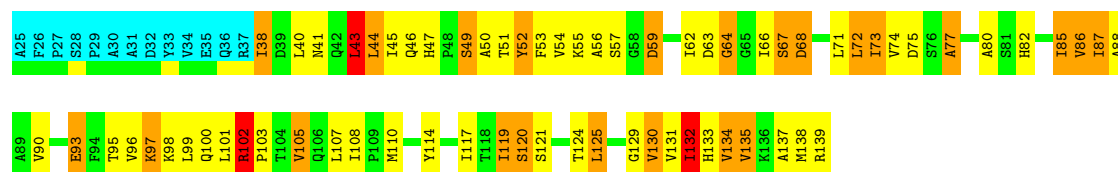


• Molecule 1: UMUD' PROTEIN

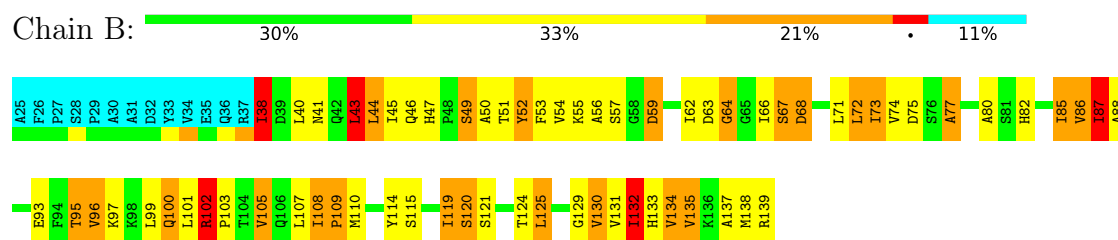


4.2.3 Score per residue for model 3

• Molecule 1: UMUD' PROTEIN

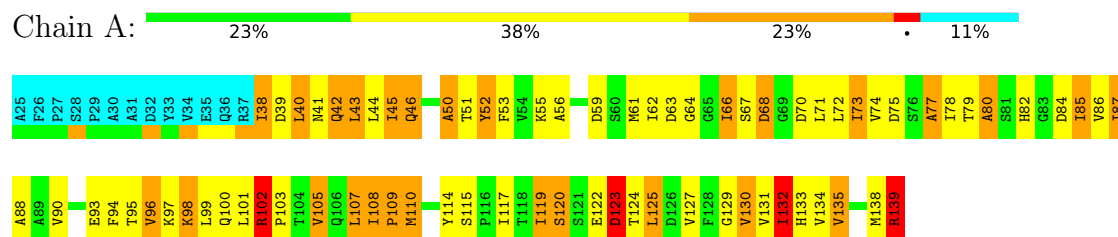


• Molecule 1: UMUD' PROTEIN

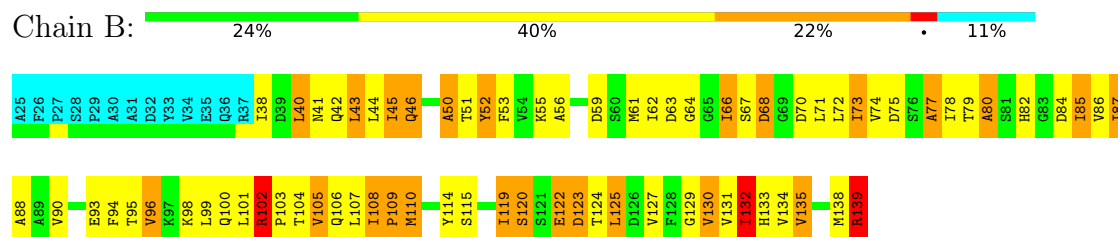


4.2.4 Score per residue for model 4

- Molecule 1: UMUD' PROTEIN

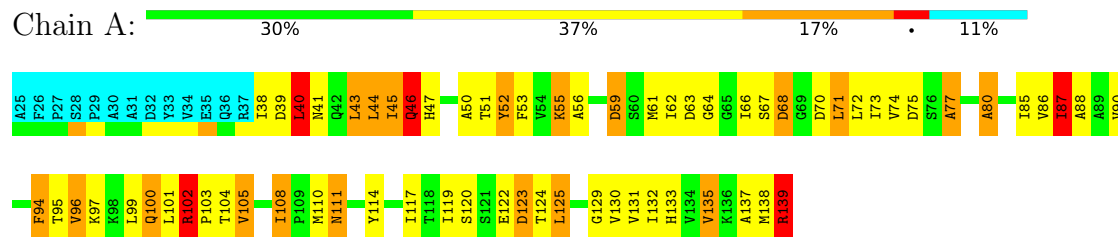


- Molecule 1: UMUD' PROTEIN

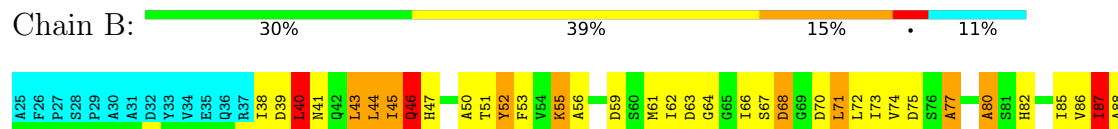


4.2.5 Score per residue for model 5

- Molecule 1: UMUD' PROTEIN



- Molecule 1: UMUD' PROTEIN





4.2.6 Score per residue for model 6 (medoid)

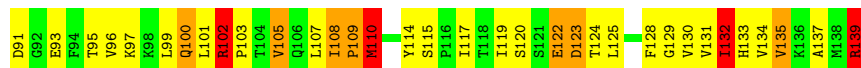
- Molecule 1: UMUD' PROTEIN

Chain A: 28% 38% 20% • 11%



- Molecule 1: UMUD' PROTEIN

Chain B: 28% 40% 17% • 11%



4.2.7 Score per residue for model 7

- Molecule 1: UMUD' PROTEIN

Chain A: 19% 44% 21% • 11%



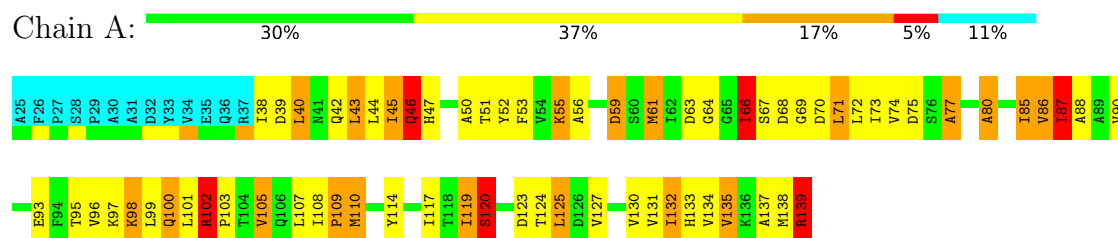
- Molecule 1: UMUD' PROTEIN

Chain B: 20% 45% 18% 5% 11%

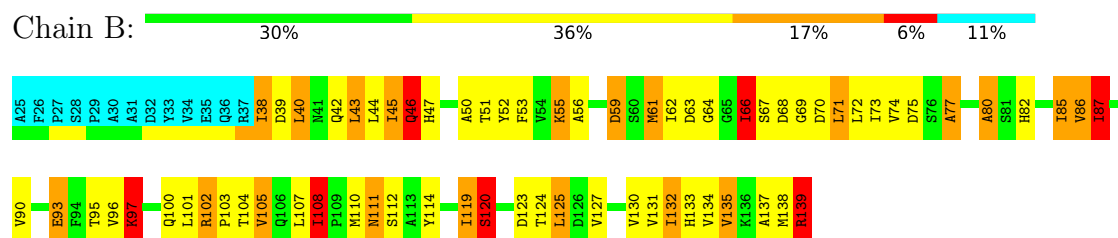


4.2.8 Score per residue for model 8

• Molecule 1: UMUD' PROTEIN

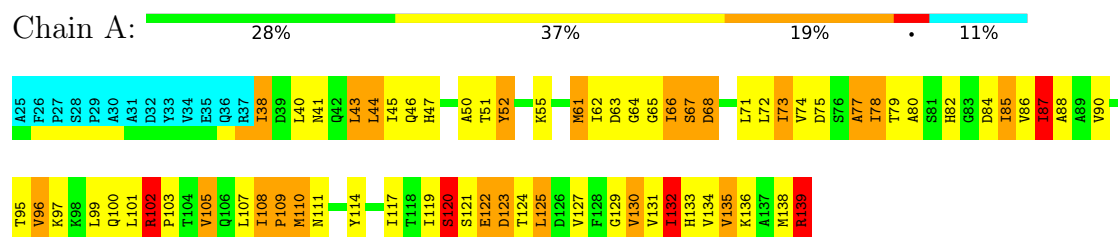


• Molecule 1: UMUD' PROTEIN

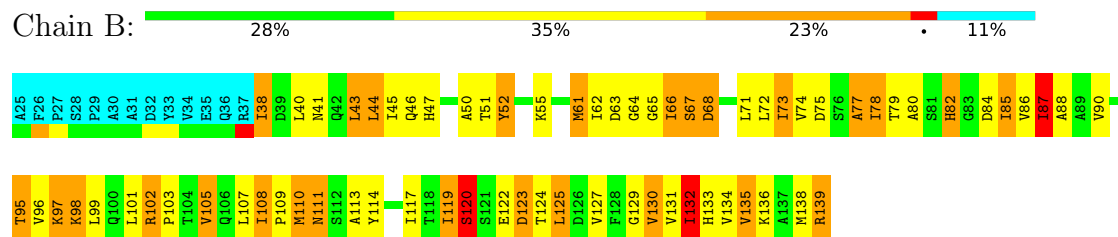


4.2.9 Score per residue for model 9

• Molecule 1: UMUD' PROTEIN



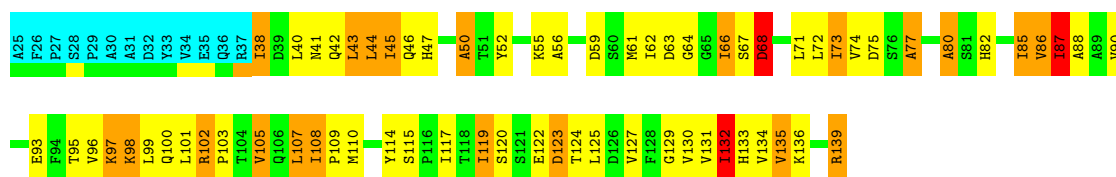
• Molecule 1: UMUD' PROTEIN



4.2.10 Score per residue for model 10

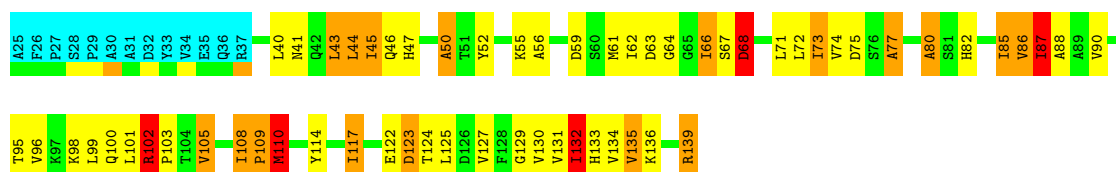
• Molecule 1: UMUD' PROTEIN





• Molecule 1: UMUD' PROTEIN

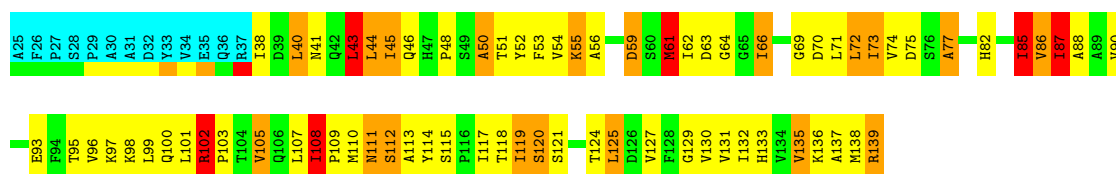
Chain B: 37% 33% 15% 11%



4.2.11 Score per residue for model 11

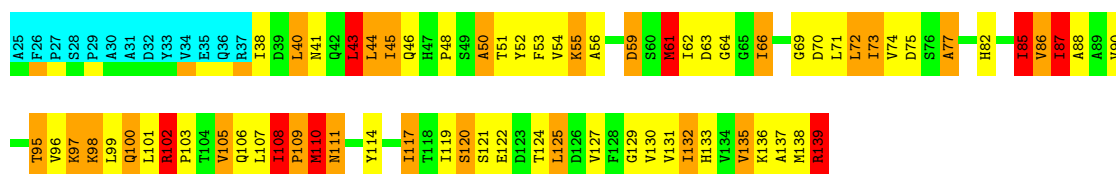
• Molecule 1: UMUD' PROTEIN

Chain A: 25% 42% 17% 5% 11%



• Molecule 1: UMUD' PROTEIN

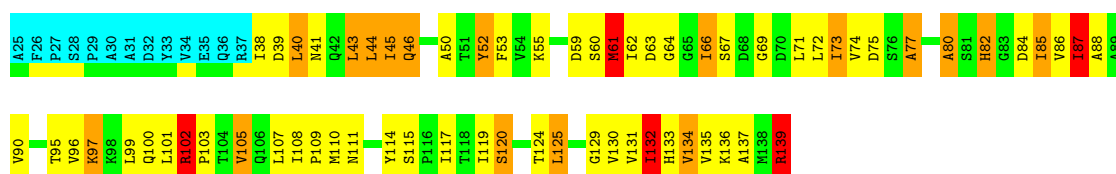
Chain B: 28% 34% 20% 7% 11%



4.2.12 Score per residue for model 12

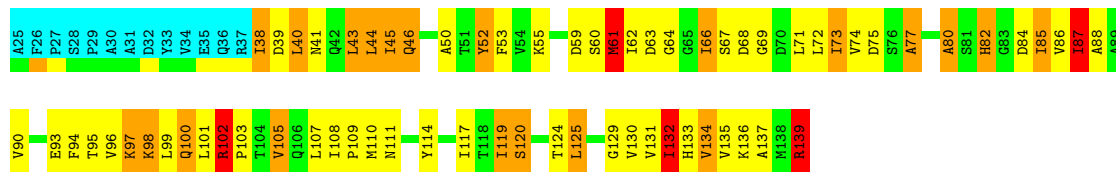
• Molecule 1: UMUD' PROTEIN

Chain A: 31% 38% 15% 11%



- Molecule 1: UMUD' PROTEIN

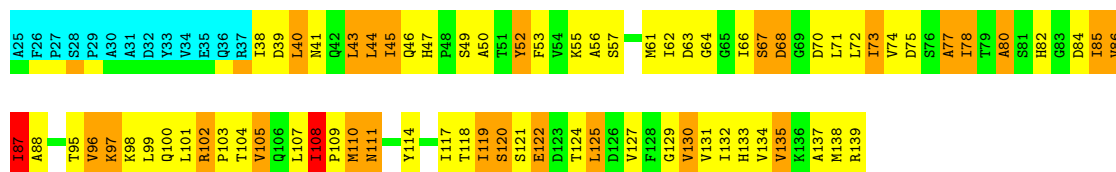
Chain B:



4.2.13 Score per residue for model 13

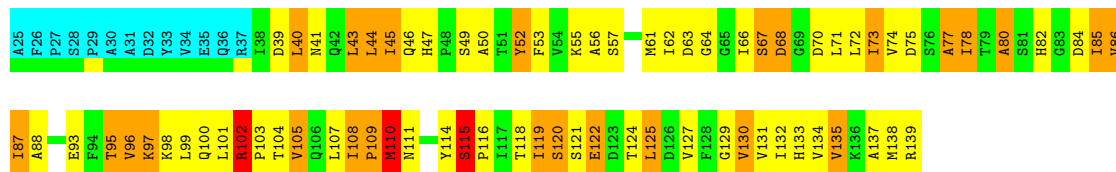
- Molecule 1: UMUD' PROTEIN

Chain A:



- Molecule 1: UMUD' PROTEIN

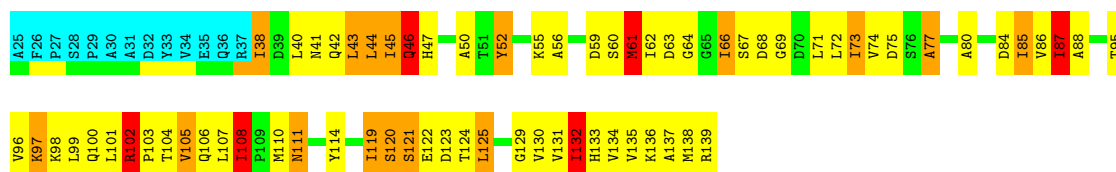
Chain B:



4.2.14 Score per residue for model 14

- Molecule 1: UMUD' PROTEIN

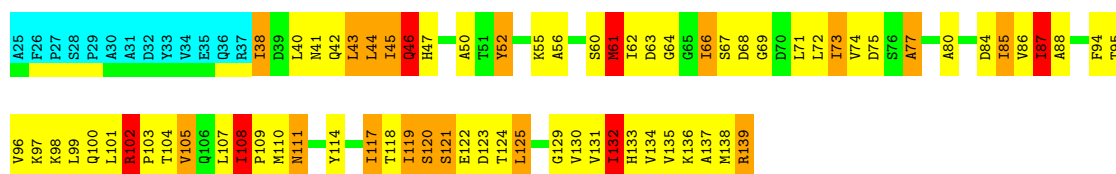
Chain A:



- Molecule 1: UMUD' PROTEIN

Chain B:

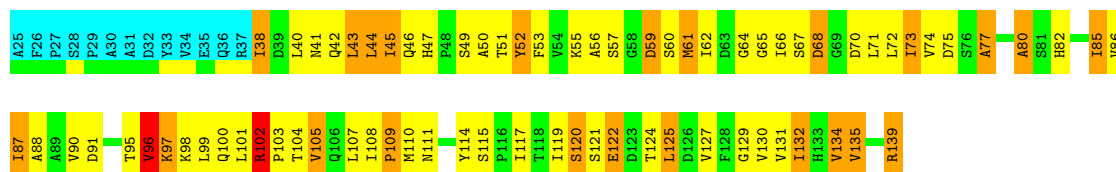




4.2.15 Score per residue for model 15

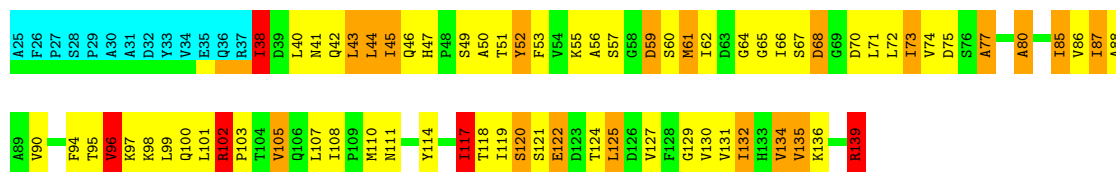
• Molecule 1: UMUD' PROTEIN

Chain A: 24% 43% 20% 11%



• Molecule 1: UMUD' PROTEIN

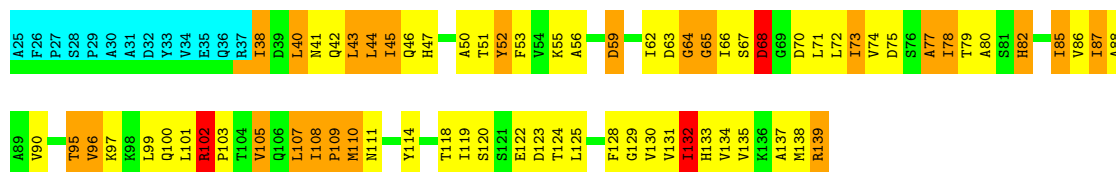
Chain B: 26% 42% 17% 11%



4.2.16 Score per residue for model 16

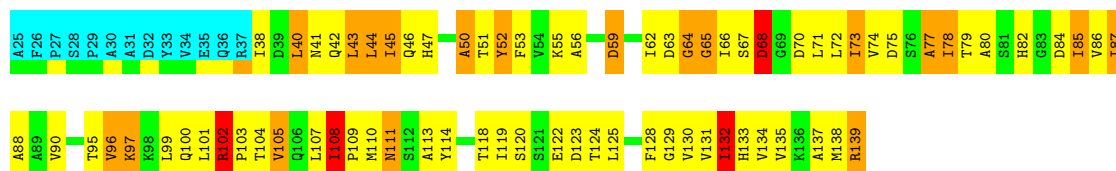
• Molecule 1: UMUD' PROTEIN

Chain A: 26% 40% 20% 11%



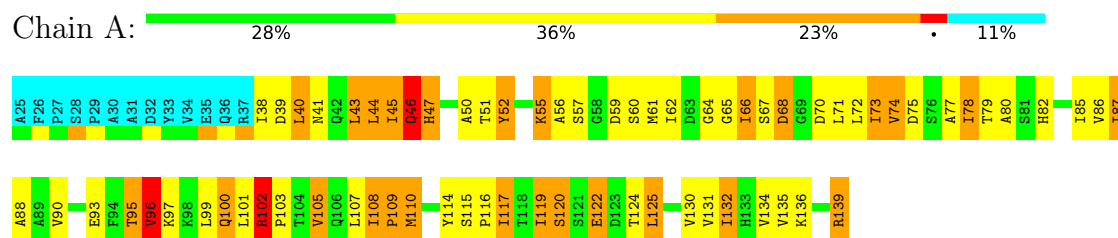
• Molecule 1: UMUD' PROTEIN

Chain B: 23% 45% 17% 11%

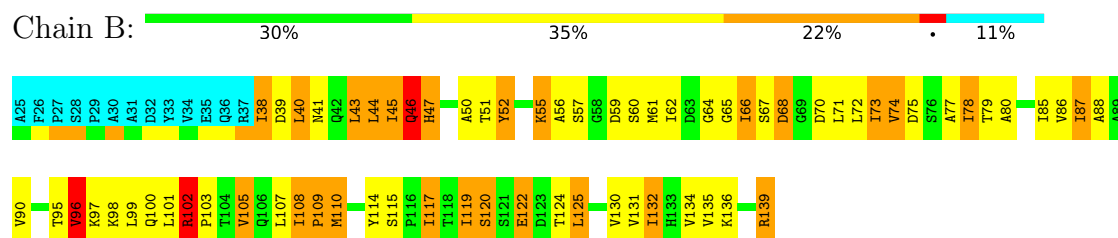


4.2.17 Score per residue for model 17

• Molecule 1: UMUD' PROTEIN

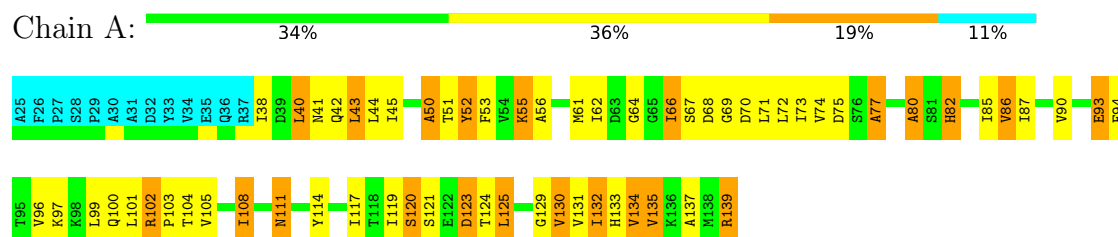


• Molecule 1: UMUD' PROTEIN

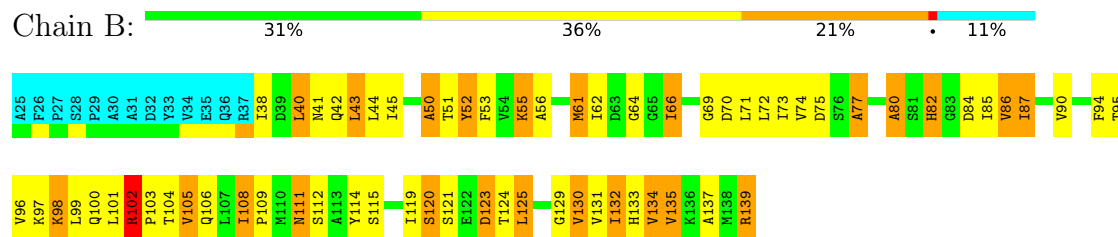


4.2.18 Score per residue for model 18

• Molecule 1: UMUD' PROTEIN



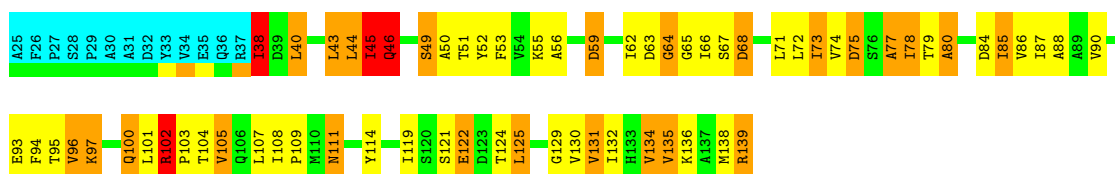
• Molecule 1: UMUD' PROTEIN



4.2.19 Score per residue for model 19

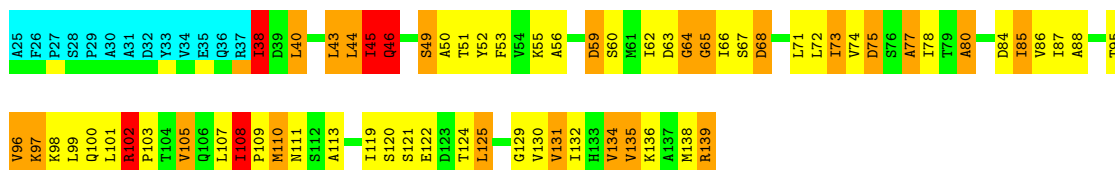
• Molecule 1: UMUD' PROTEIN





• Molecule 1: UMUD' PROTEIN

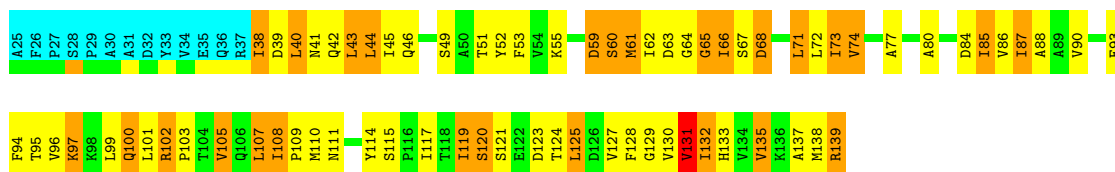
Chain B: 31% 34% 19% • 11%



4.2.20 Score per residue for model 20

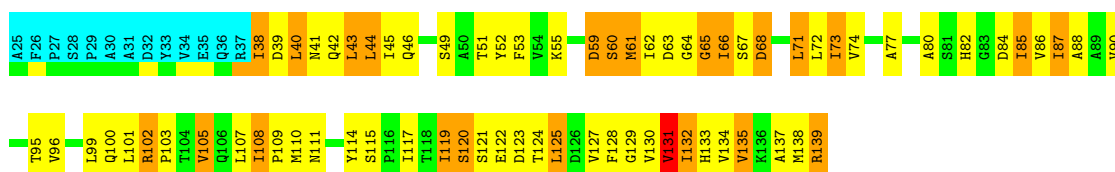
• Molecule 1: UMUD' PROTEIN

Chain A: 26% 38% 23% • 11%



• Molecule 1: UMUD' PROTEIN

Chain B: 26% 42% 20% • 11%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.851

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.44±0.01	0±0/774 (0.0± 0.0%)	1.65±0.02	8±2/1052 (0.7± 0.2%)
1	B	1.45±0.01	0±0/774 (0.0± 0.0%)	1.65±0.02	8±2/1052 (0.8± 0.2%)
All	All	1.45	0/30960 (0.0%)	1.65	320/42080 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
1	B	0.0±0.0	2.0±0.0
All	All	0	80

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	132	ILE	N-CA-CB	-7.96	104.69	112.65	11	1
1	A	131	VAL	N-CA-CB	-7.80	104.84	112.65	20	2
1	B	131	VAL	N-CA-CB	-7.73	104.92	112.65	20	2
1	B	96	VAL	N-CA-CB	-7.16	105.49	112.65	6	3
1	A	119	ILE	N-CA-CB	-6.99	104.37	112.34	7	10
1	B	45	ILE	N-CA-CB	-6.92	104.45	112.34	2	7
1	B	119	ILE	N-CA-CB	-6.92	104.45	112.34	7	11
1	A	45	ILE	N-CA-CB	-6.87	104.51	112.34	2	7
1	A	96	VAL	N-CA-CB	-6.79	105.86	112.65	6	5
1	B	73	ILE	N-CA-CB	-6.61	104.49	112.35	4	15
1	A	73	ILE	N-CA-CB	-6.59	104.51	112.35	1	15
1	B	86	VAL	N-CA-CB	-6.57	104.58	112.07	18	8
1	A	86	VAL	N-CA-CB	-6.52	104.64	112.07	18	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	105	VAL	N-CA-CB	-6.48	104.90	111.90	18	19
1	A	78	ILE	N-CA-CB	-6.41	105.03	112.34	6	7
1	B	78	ILE	N-CA-CB	-6.40	105.04	112.34	6	7
1	A	105	VAL	N-CA-CB	-6.37	105.02	111.90	9	19
1	A	135	VAL	N-CA-CB	-6.32	104.83	112.35	11	20
1	A	66	ILE	N-CA-CB	-6.31	105.08	111.90	8	10
1	B	66	ILE	N-CA-CB	-6.31	105.08	111.90	8	10
1	B	135	VAL	N-CA-CB	-6.20	104.97	112.35	11	20
1	B	38	ILE	N-CA-CB	-6.08	105.12	112.35	11	1
1	A	50	ALA	N-CA-CB	-5.95	104.65	111.79	18	4
1	B	50	ALA	N-CA-CB	-5.91	104.69	111.79	18	5
1	A	38	ILE	N-CA-CB	-5.91	104.92	111.66	6	3
1	B	49	SER	N-CA-CB	-5.68	104.97	111.79	3	1
1	A	49	SER	N-CA-CB	-5.66	105.00	111.79	3	1
1	B	108	ILE	N-CA-CB	-5.61	103.35	111.21	19	5
1	B	61	MET	N-CA-CB	-5.56	105.12	111.79	12	1
1	B	74	VAL	N-CA-CB	-5.45	104.56	111.64	17	1
1	A	61	MET	N-CA-CB	-5.45	105.26	111.79	12	1
1	A	74	VAL	N-CA-CB	-5.43	104.58	111.64	17	2
1	B	43	LEU	N-CA-CB	-5.41	102.57	110.47	11	2
1	B	117	ILE	N-CA-CB	-5.41	104.61	111.64	15	4
1	A	134	VAL	N-CA-CB	-5.40	104.89	111.21	4	15
1	A	43	LEU	N-CA-CB	-5.39	102.60	110.47	11	2
1	B	134	VAL	N-CA-CB	-5.35	104.95	111.21	4	16
1	A	82	HIS	CA-CB-CG	-5.34	108.46	113.80	7	10
1	A	117	ILE	N-CA-CB	-5.31	105.00	110.95	7	2
1	A	108	ILE	N-CA-CB	-5.30	103.79	111.21	13	4
1	B	82	HIS	CA-CB-CG	-5.30	108.50	113.80	12	10
1	A	87	ILE	N-CA-CB	-5.19	105.09	111.00	1	10
1	B	87	ILE	N-CA-CB	-5.18	105.10	111.00	14	13
1	B	91	ASP	N-CA-CB	-5.03	104.79	112.28	7	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	102	ARG	Sidechain	20
1	A	139	ARG	Sidechain	20
1	B	102	ARG	Sidechain	20
1	B	139	ARG	Sidechain	20

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	763	778	778	106±9
1	B	763	778	778	107±11
All	All	30520	31120	31120	3696

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HD11	1:B:40:LEU:HD13	1.05	1.27	11	3
1:A:44:LEU:HD23	1:B:44:LEU:HD23	1.04	1.20	8	12
1:B:107:LEU:HD13	1:B:119:ILE:HD11	1.01	1.26	11	2
1:A:40:LEU:HD13	1:B:45:ILE:HD11	1.00	1.29	11	3
1:B:95:THR:HG21	1:B:107:LEU:HD23	1.00	1.29	9	2
1:A:72:LEU:HD11	1:A:132:ILE:HG23	0.96	1.37	10	3
1:A:45:ILE:HD12	1:B:40:LEU:HD13	0.95	1.38	13	1
1:A:40:LEU:HD13	1:B:45:ILE:HD12	0.95	1.38	13	1
1:B:72:LEU:HD11	1:B:132:ILE:HG23	0.94	1.37	10	3
1:A:135:VAL:HG12	1:B:133:HIS:CD2	0.94	1.98	2	1
1:A:133:HIS:CD2	1:B:135:VAL:HG12	0.93	1.98	2	1
1:A:135:VAL:HG22	1:B:135:VAL:HG22	0.93	1.39	10	8
1:A:88:ALA:HB3	1:A:95:THR:CG2	0.91	1.95	2	1
1:B:43:LEU:HD13	1:B:44:LEU:N	0.91	1.80	13	3
1:A:40:LEU:HD23	1:B:40:LEU:HD23	0.90	1.42	18	2
1:A:43:LEU:HD13	1:A:44:LEU:N	0.90	1.80	13	3
1:B:45:ILE:HD13	1:B:51:THR:HG21	0.89	1.44	17	4
1:A:40:LEU:HD11	1:B:45:ILE:HD11	0.89	1.43	7	4
1:A:40:LEU:HD12	1:B:45:ILE:HD13	0.89	1.43	2	1
1:A:135:VAL:HG22	1:B:135:VAL:HG13	0.89	1.45	5	9
1:B:95:THR:HG21	1:B:107:LEU:HD11	0.89	1.43	5	1
1:A:45:ILE:HD13	1:B:40:LEU:HD12	0.88	1.44	2	1
1:A:43:LEU:CD1	1:A:44:LEU:HD22	0.88	1.98	11	2
1:B:43:LEU:CD1	1:B:44:LEU:HD22	0.88	1.98	11	2
1:A:66:ILE:HG23	1:A:72:LEU:HD12	0.88	1.45	5	6
1:B:66:ILE:HG23	1:B:72:LEU:HD12	0.88	1.43	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HD12	1:A:111:ASN:ND2	0.88	1.82	18	3
1:A:40:LEU:CD1	1:A:44:LEU:HD22	0.88	1.98	8	3
1:A:40:LEU:CD1	1:B:45:ILE:HD11	0.87	1.99	4	5
1:A:107:LEU:HD23	1:A:119:ILE:HD11	0.87	1.43	14	1
1:A:72:LEU:HD13	1:A:73:ILE:N	0.87	1.84	17	4
1:A:135:VAL:HG13	1:B:135:VAL:HG22	0.87	1.45	5	8
1:B:62:ILE:HD12	1:B:111:ASN:ND2	0.87	1.85	18	5
1:A:45:ILE:HD11	1:B:40:LEU:CD1	0.87	2.00	4	5
1:A:107:LEU:HD13	1:A:119:ILE:HD11	0.87	1.46	11	1
1:A:45:ILE:HD13	1:A:51:THR:HG21	0.87	1.44	17	4
1:B:72:LEU:HD23	1:B:73:ILE:N	0.87	1.85	6	14
1:B:88:ALA:HB3	1:B:95:THR:OG1	0.87	1.70	11	15
1:B:40:LEU:CD1	1:B:44:LEU:HD22	0.86	1.99	8	3
1:B:62:ILE:HD12	1:B:111:ASN:CG	0.86	1.96	9	11
1:A:88:ALA:HB3	1:A:95:THR:OG1	0.86	1.71	20	14
1:B:43:LEU:HD11	1:B:44:LEU:HD22	0.86	1.46	11	2
1:B:72:LEU:HD13	1:B:73:ILE:N	0.86	1.85	17	4
1:A:45:ILE:HD11	1:B:40:LEU:HD11	0.85	1.43	7	4
1:A:44:LEU:HD23	1:B:44:LEU:CD2	0.85	2.02	18	5
1:A:43:LEU:HD11	1:A:44:LEU:HD22	0.85	1.46	11	2
1:A:44:LEU:CD2	1:B:44:LEU:HD23	0.85	2.02	18	5
1:B:38:ILE:HD12	1:B:40:LEU:HD23	0.85	1.49	12	1
1:A:72:LEU:HD23	1:A:73:ILE:N	0.84	1.85	6	14
1:B:99:LEU:HD12	1:B:101:LEU:HD21	0.83	1.51	1	8
1:A:64:GLY:O	1:A:96:VAL:HG11	0.83	1.73	3	2
1:B:72:LEU:HD12	1:B:73:ILE:N	0.83	1.88	3	1
1:A:72:LEU:HD12	1:A:73:ILE:N	0.82	1.88	3	1
1:B:107:LEU:HD13	1:B:119:ILE:HD12	0.82	1.50	7	1
1:A:43:LEU:HD13	1:A:44:LEU:HD13	0.82	1.52	10	2
1:A:62:ILE:HG23	1:A:67:SER:OG	0.82	1.74	16	2
1:B:95:THR:HG21	1:B:107:LEU:CD2	0.82	2.04	9	4
1:A:80:ALA:HB1	1:A:86:VAL:HG11	0.81	1.53	4	14
1:A:41:ASN:CB	1:B:40:LEU:HD13	0.81	2.05	5	1
1:A:100:GLN:O	1:A:101:LEU:HD23	0.81	1.73	20	17
1:A:40:LEU:HD13	1:B:41:ASN:CB	0.81	2.04	5	1
1:A:131:VAL:C	1:A:132:ILE:HD12	0.81	2.01	11	17
1:B:43:LEU:HD22	1:B:43:LEU:O	0.81	1.76	11	2
1:B:131:VAL:C	1:B:132:ILE:HD12	0.81	2.01	11	17
1:B:62:ILE:HG23	1:B:67:SER:OG	0.81	1.76	16	2
1:A:40:LEU:HD12	1:A:41:ASN:N	0.81	1.90	15	4
1:B:80:ALA:HB1	1:B:86:VAL:HG11	0.81	1.53	4	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD12	1:B:41:ASN:N	0.80	1.91	3	4
1:A:101:LEU:HD12	1:A:102:ARG:N	0.80	1.91	7	1
1:A:106:GLN:O	1:A:107:LEU:HD12	0.80	1.76	7	1
1:B:43:LEU:HD13	1:B:44:LEU:HD13	0.80	1.52	10	2
1:A:43:LEU:HD22	1:A:43:LEU:O	0.80	1.76	11	2
1:A:132:ILE:HG23	1:B:138:MET:O	0.80	1.75	20	1
1:A:45:ILE:HD13	1:A:51:THR:CG2	0.79	2.08	17	3
1:A:138:MET:O	1:B:132:ILE:HG23	0.79	1.75	20	1
1:A:45:ILE:CD1	1:B:40:LEU:HD13	0.79	2.07	13	4
1:B:80:ALA:CB	1:B:86:VAL:HG11	0.78	2.08	10	16
1:A:43:LEU:HD21	1:B:71:LEU:HD11	0.78	1.53	3	1
1:A:62:ILE:HD12	1:A:111:ASN:CG	0.78	2.03	13	9
1:A:80:ALA:CB	1:A:86:VAL:HG11	0.78	2.08	10	15
1:B:100:GLN:O	1:B:101:LEU:HD23	0.78	1.78	6	18
1:A:71:LEU:HD11	1:B:43:LEU:HD21	0.78	1.53	3	1
1:A:40:LEU:HD13	1:B:45:ILE:CD1	0.78	2.07	13	4
1:B:45:ILE:HD13	1:B:51:THR:CG2	0.78	2.07	17	3
1:B:63:ASP:OD2	1:B:108:ILE:HD11	0.78	1.77	13	3
1:B:85:ILE:O	1:B:132:ILE:HD13	0.77	1.79	12	12
1:B:64:GLY:O	1:B:96:VAL:HG11	0.77	1.78	3	2
1:A:40:LEU:HD11	1:B:45:ILE:HD12	0.77	1.53	16	3
1:A:44:LEU:HD11	1:B:73:ILE:HD11	0.77	1.56	18	7
1:A:85:ILE:O	1:A:132:ILE:HD13	0.77	1.79	12	12
1:A:41:ASN:HB3	1:B:40:LEU:HD21	0.77	1.57	2	1
1:A:45:ILE:CD1	1:B:40:LEU:HD21	0.77	2.09	8	5
1:A:40:LEU:HD21	1:B:41:ASN:HB3	0.77	1.57	2	1
1:A:40:LEU:HD21	1:B:45:ILE:CD1	0.76	2.09	8	5
1:B:88:ALA:HB3	1:B:95:THR:HB	0.76	1.56	5	2
1:A:97:LYS:HD2	1:A:107:LEU:HD12	0.76	1.56	14	1
1:A:45:ILE:HD12	1:B:40:LEU:HD11	0.76	1.53	16	3
1:A:105:VAL:HG23	1:A:118:THR:HG1	0.76	1.40	16	1
1:B:53:PHE:HB3	1:B:73:ILE:HD13	0.76	1.56	11	11
1:A:41:ASN:HA	1:B:40:LEU:HD22	0.76	1.58	18	6
1:A:73:ILE:HD11	1:B:44:LEU:HD11	0.76	1.56	8	7
1:A:53:PHE:HB3	1:A:73:ILE:HD13	0.76	1.56	11	11
1:B:64:GLY:O	1:B:85:ILE:HD11	0.76	1.81	6	5
1:A:64:GLY:O	1:A:85:ILE:HD11	0.75	1.81	6	5
1:A:44:LEU:HB3	1:B:44:LEU:HD23	0.75	1.57	9	8
1:A:82:HIS:NE2	1:A:101:LEU:HD11	0.75	1.97	7	1
1:B:95:THR:HG23	1:B:109:PRO:HB3	0.75	1.58	12	1
1:B:101:LEU:HD13	1:B:125:LEU:O	0.75	1.82	19	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:64:GLY:HA3	1:B:96:VAL:HG11	0.74	1.58	15	7
1:B:105:VAL:HG11	1:B:120:SER:O	0.74	1.82	11	5
1:A:105:VAL:HG11	1:A:122:GLU:N	0.74	1.97	16	5
1:A:44:LEU:HD23	1:B:44:LEU:HB3	0.74	1.57	9	6
1:B:87:ILE:O	1:B:127:VAL:HG13	0.74	1.83	20	4
1:A:105:VAL:HG23	1:A:118:THR:OG1	0.74	1.81	16	3
1:A:97:LYS:CD	1:A:107:LEU:HD12	0.74	2.12	14	1
1:B:110:MET:O	1:B:110:MET:HE3	0.74	1.83	15	2
1:A:87:ILE:O	1:A:127:VAL:HG13	0.74	1.83	20	4
1:A:45:ILE:HD12	1:B:40:LEU:CD1	0.74	2.13	13	3
1:B:45:ILE:CD1	1:B:51:THR:HG21	0.74	2.13	17	1
1:A:132:ILE:HG23	1:B:138:MET:C	0.73	2.08	20	1
1:A:40:LEU:HD22	1:B:41:ASN:HA	0.73	1.58	18	6
1:A:138:MET:C	1:B:132:ILE:HG23	0.73	2.07	20	1
1:A:40:LEU:CD1	1:B:45:ILE:HD12	0.73	2.13	13	3
1:A:105:VAL:HG11	1:A:120:SER:O	0.73	1.84	11	3
1:B:62:ILE:HD12	1:B:111:ASN:OD1	0.73	1.82	11	5
1:A:139:ARG:OXT	1:B:85:ILE:HG22	0.72	1.84	8	1
1:A:45:ILE:CD1	1:A:51:THR:HG21	0.72	2.13	17	1
1:B:45:ILE:HG23	1:B:51:THR:HG21	0.72	1.60	15	5
1:B:106:GLN:O	1:B:107:LEU:HD12	0.72	1.84	7	1
1:B:75:ASP:HB3	1:B:131:VAL:HG12	0.72	1.62	3	2
1:A:45:ILE:HG21	1:A:51:THR:OG1	0.72	1.85	4	2
1:A:61:MET:HG2	1:A:96:VAL:HG21	0.71	1.60	7	2
1:B:86:VAL:HG12	1:B:130:VAL:HG13	0.71	1.62	20	1
1:B:45:ILE:HG21	1:B:51:THR:OG1	0.71	1.85	4	2
1:A:40:LEU:HD13	1:B:41:ASN:HB3	0.71	1.61	5	1
1:A:133:HIS:NE2	1:B:137:ALA:HB1	0.71	2.01	20	1
1:A:62:ILE:HG23	1:A:67:SER:HB2	0.71	1.62	15	1
1:B:75:ASP:HB2	1:B:131:VAL:HG12	0.71	1.63	12	16
1:B:62:ILE:HG23	1:B:67:SER:HB2	0.71	1.63	15	1
1:A:41:ASN:HB3	1:B:40:LEU:HD13	0.71	1.61	5	1
1:A:45:ILE:HG23	1:A:51:THR:HG21	0.71	1.60	15	5
1:A:137:ALA:HB1	1:B:133:HIS:NE2	0.71	2.00	20	1
1:A:40:LEU:CD2	1:B:40:LEU:HD23	0.70	2.16	18	1
1:A:40:LEU:HD23	1:B:40:LEU:CD2	0.70	2.16	18	1
1:A:64:GLY:CA	1:A:96:VAL:HG11	0.70	2.15	18	4
1:A:71:LEU:HD13	1:A:72:LEU:N	0.70	2.02	19	2
1:A:88:ALA:HB3	1:A:95:THR:HG23	0.70	1.62	2	1
1:A:90:VAL:HB	1:A:125:LEU:HD22	0.70	1.62	12	5
1:B:99:LEU:CB	1:B:107:LEU:HD12	0.70	2.16	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HD12	1:A:111:ASN:OD1	0.70	1.86	16	8
1:A:108:ILE:O	1:A:108:ILE:HD13	0.70	1.86	18	2
1:B:61:MET:N	1:B:66:ILE:HD11	0.70	2.01	14	6
1:A:64:GLY:HA3	1:A:96:VAL:HG11	0.70	1.63	15	9
1:A:75:ASP:HB3	1:A:131:VAL:HG12	0.70	1.62	3	2
1:B:90:VAL:HB	1:B:125:LEU:HD22	0.70	1.62	12	4
1:A:85:ILE:HG22	1:B:139:ARG:OXT	0.70	1.86	8	1
1:A:75:ASP:N	1:A:131:VAL:HG12	0.70	2.02	19	1
1:B:50:ALA:HB1	1:B:77:ALA:HB2	0.69	1.65	12	17
1:A:86:VAL:HG12	1:A:130:VAL:HG13	0.69	1.63	20	1
1:A:47:HIS:CB	1:A:50:ALA:HB3	0.69	2.18	9	2
1:B:47:HIS:CB	1:B:50:ALA:HB3	0.69	2.18	9	3
1:B:71:LEU:HD13	1:B:72:LEU:N	0.69	2.02	19	2
1:B:108:ILE:HD13	1:B:108:ILE:O	0.69	1.88	1	3
1:B:75:ASP:N	1:B:131:VAL:HG12	0.69	2.02	19	1
1:A:61:MET:N	1:A:66:ILE:HD11	0.69	2.03	14	6
1:A:75:ASP:HB2	1:A:131:VAL:HG12	0.69	1.63	12	16
1:A:110:MET:HE3	1:A:110:MET:O	0.69	1.87	3	2
1:A:99:LEU:CB	1:A:107:LEU:HD12	0.69	2.18	16	5
1:A:45:ILE:HG13	1:B:40:LEU:HD21	0.69	1.63	17	3
1:B:72:LEU:CD1	1:B:132:ILE:HG23	0.69	2.17	10	1
1:A:45:ILE:CG1	1:B:40:LEU:HD21	0.69	2.17	17	3
1:A:72:LEU:CD1	1:A:132:ILE:HG23	0.68	2.16	10	1
1:B:64:GLY:CA	1:B:96:VAL:HG11	0.68	2.18	18	3
1:A:59:ASP:CA	1:A:62:ILE:HD11	0.68	2.19	3	9
1:B:59:ASP:CA	1:B:62:ILE:HD11	0.68	2.18	3	10
1:A:40:LEU:HD21	1:B:45:ILE:CG1	0.68	2.17	17	3
1:B:62:ILE:HD12	1:B:111:ASN:HD21	0.68	1.48	18	3
1:A:44:LEU:CD1	1:B:71:LEU:HD12	0.68	2.18	16	11
1:A:50:ALA:HB1	1:A:77:ALA:HB2	0.68	1.65	9	17
1:A:66:ILE:CG2	1:A:72:LEU:HD12	0.68	2.19	18	7
1:A:137:ALA:HB2	1:B:133:HIS:CE1	0.67	2.24	2	1
1:B:99:LEU:HB3	1:B:107:LEU:HD12	0.67	1.66	3	4
1:A:133:HIS:CE1	1:B:137:ALA:HB2	0.67	2.24	2	1
1:B:119:ILE:HD13	1:B:125:LEU:HG	0.67	1.64	14	6
1:B:38:ILE:CD1	1:B:40:LEU:HD23	0.67	2.19	12	1
1:A:62:ILE:HD12	1:A:111:ASN:HD21	0.67	1.50	18	2
1:B:66:ILE:CG2	1:B:72:LEU:HD12	0.67	2.19	5	6
1:B:66:ILE:HD12	1:B:66:ILE:O	0.67	1.90	3	20
1:A:40:LEU:HD21	1:B:45:ILE:HG13	0.67	1.64	17	3
1:A:71:LEU:HD12	1:B:44:LEU:CD1	0.67	2.18	16	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:ASP:O	1:B:43:LEU:HD12	0.67	1.89	13	1
1:A:66:ILE:HD12	1:A:66:ILE:O	0.67	1.89	3	19
1:A:47:HIS:HB3	1:A:50:ALA:HB3	0.67	1.66	6	7
1:A:71:LEU:HD12	1:B:44:LEU:HD11	0.67	1.66	9	7
1:B:47:HIS:HB3	1:B:50:ALA:HB3	0.66	1.66	6	7
1:B:72:LEU:HD21	1:B:132:ILE:CG2	0.66	2.20	10	3
1:A:43:LEU:HD13	1:A:43:LEU:C	0.66	2.15	11	3
1:A:71:LEU:HD11	1:A:73:ILE:HD11	0.66	1.67	3	4
1:A:99:LEU:HD21	1:A:127:VAL:HG22	0.66	1.67	13	1
1:B:74:VAL:HG23	1:B:131:VAL:HB	0.66	1.67	20	1
1:B:71:LEU:HD11	1:B:73:ILE:HD11	0.66	1.68	3	4
1:A:74:VAL:HG23	1:A:131:VAL:HB	0.66	1.67	20	1
1:A:85:ILE:O	1:A:85:ILE:HG23	0.66	1.91	8	20
1:B:43:LEU:HD13	1:B:43:LEU:C	0.66	2.15	11	3
1:B:43:LEU:HD22	1:B:43:LEU:C	0.66	2.15	11	2
1:B:80:ALA:HB2	1:B:130:VAL:HA	0.66	1.67	6	7
1:A:64:GLY:HA2	1:A:85:ILE:HD11	0.66	1.65	5	5
1:B:85:ILE:O	1:B:85:ILE:HG23	0.66	1.90	11	19
1:A:119:ILE:HD13	1:A:125:LEU:HG	0.66	1.68	2	5
1:A:43:LEU:HD22	1:A:43:LEU:C	0.66	2.14	11	2
1:A:99:LEU:HD12	1:A:101:LEU:HD21	0.66	1.67	4	6
1:B:40:LEU:HD12	1:B:40:LEU:C	0.66	2.15	9	3
1:A:45:ILE:HD12	1:B:40:LEU:CG	0.66	2.21	16	4
1:B:131:VAL:O	1:B:132:ILE:HD13	0.66	1.91	13	2
1:A:40:LEU:CG	1:B:45:ILE:HD12	0.66	2.21	16	4
1:A:131:VAL:O	1:A:132:ILE:HD13	0.65	1.91	13	2
1:A:44:LEU:HD11	1:B:71:LEU:HD12	0.65	1.66	9	7
1:A:99:LEU:HB2	1:A:107:LEU:HD12	0.65	1.66	16	5
1:A:40:LEU:HD13	1:B:41:ASN:HA	0.65	1.67	15	4
1:A:108:ILE:C	1:A:108:ILE:HD13	0.65	2.16	1	2
1:B:64:GLY:HA2	1:B:85:ILE:HD11	0.65	1.66	5	5
1:A:73:ILE:HD11	1:B:43:LEU:CD1	0.65	2.21	4	6
1:A:72:LEU:HD21	1:A:132:ILE:CG2	0.65	2.20	10	3
1:A:105:VAL:HG12	1:A:119:ILE:HB	0.65	1.68	2	2
1:A:43:LEU:CD1	1:B:73:ILE:HD11	0.65	2.22	4	6
1:A:44:LEU:HD23	1:B:44:LEU:HB2	0.65	1.66	2	4
1:A:44:LEU:HB2	1:B:44:LEU:HD23	0.65	1.67	2	4
1:B:61:MET:HG2	1:B:96:VAL:HG21	0.65	1.69	9	2
1:A:131:VAL:HG21	1:A:133:HIS:NE2	0.65	2.07	1	4
1:A:80:ALA:HB2	1:A:130:VAL:HA	0.65	1.67	6	7
1:A:124:THR:C	1:A:125:LEU:HD22	0.65	2.17	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:99:LEU:HB2	1:B:107:LEU:HD12	0.65	1.69	14	5
1:B:88:ALA:HB2	1:B:99:LEU:HD22	0.65	1.67	7	1
1:B:108:ILE:C	1:B:108:ILE:HD13	0.65	2.16	18	4
1:A:39:ASP:O	1:A:43:LEU:HD12	0.65	1.92	13	1
1:A:105:VAL:HG11	1:A:122:GLU:H	0.64	1.52	19	5
1:A:60:SER:O	1:A:61:MET:HE3	0.64	1.92	12	2
1:A:84:ASP:O	1:A:86:VAL:HG22	0.64	1.93	7	2
1:A:41:ASN:HA	1:B:40:LEU:HD13	0.64	1.68	15	4
1:B:52:TYR:O	1:B:74:VAL:HG12	0.64	1.92	2	19
1:B:124:THR:C	1:B:125:LEU:HD22	0.64	2.17	10	4
1:A:99:LEU:HD22	1:A:127:VAL:CG2	0.64	2.23	7	1
1:A:138:MET:HB3	1:B:85:ILE:HD13	0.64	1.68	13	1
1:A:52:TYR:O	1:A:74:VAL:HG12	0.64	1.92	2	19
1:A:108:ILE:HD13	1:A:116:PRO:N	0.64	2.08	2	3
1:A:107:LEU:O	1:A:117:ILE:HG22	0.64	1.91	13	1
1:B:131:VAL:HG21	1:B:133:HIS:NE2	0.64	2.07	1	4
1:A:40:LEU:C	1:A:40:LEU:HD12	0.64	2.16	9	2
1:A:85:ILE:HD13	1:B:138:MET:HB3	0.64	1.69	13	1
1:A:71:LEU:C	1:A:71:LEU:HD13	0.64	2.18	3	14
1:B:61:MET:H	1:B:66:ILE:HD11	0.64	1.53	1	9
1:B:71:LEU:HD13	1:B:71:LEU:C	0.64	2.18	3	15
1:A:61:MET:CG	1:A:96:VAL:HG21	0.64	2.22	7	1
1:A:105:VAL:HG11	1:A:119:ILE:O	0.64	1.92	7	1
1:A:132:ILE:HD12	1:A:132:ILE:N	0.64	2.08	19	1
1:B:84:ASP:O	1:B:86:VAL:HG22	0.63	1.93	9	2
1:B:105:VAL:HG22	1:B:119:ILE:HB	0.63	1.70	18	2
1:A:64:GLY:HA2	1:A:96:VAL:HG11	0.63	1.71	18	1
1:B:61:MET:SD	1:B:95:THR:HG22	0.63	2.33	18	1
1:A:45:ILE:HD11	1:B:40:LEU:HD21	0.63	1.70	1	4
1:B:105:VAL:HG21	1:B:120:SER:O	0.63	1.94	20	5
1:A:105:VAL:HG13	1:A:105:VAL:O	0.63	1.92	7	1
1:A:105:VAL:O	1:A:105:VAL:HG13	0.63	1.93	20	2
1:A:131:VAL:HG23	1:B:139:ARG:HB3	0.63	1.69	5	7
1:B:95:THR:HG23	1:B:109:PRO:HG3	0.63	1.70	5	1
1:A:139:ARG:HB3	1:B:131:VAL:HG23	0.63	1.70	5	7
1:A:85:ILE:C	1:A:85:ILE:HD13	0.63	2.19	10	5
1:A:72:LEU:HD23	1:A:72:LEU:N	0.63	2.09	11	1
1:A:40:LEU:HD21	1:B:45:ILE:HD11	0.63	1.69	1	4
1:A:101:LEU:HD13	1:A:125:LEU:O	0.63	1.94	18	11
1:B:60:SER:O	1:B:61:MET:HE3	0.63	1.94	12	2
1:B:85:ILE:C	1:B:85:ILE:HD13	0.63	2.19	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:132:ILE:HD12	1:B:132:ILE:N	0.63	2.09	19	1
1:A:64:GLY:C	1:A:96:VAL:HG11	0.62	2.18	3	2
1:A:99:LEU:HB3	1:A:107:LEU:HD12	0.62	1.70	4	1
1:B:108:ILE:HG23	1:B:108:ILE:O	0.62	1.94	7	10
1:A:82:HIS:CE1	1:A:101:LEU:HD11	0.62	2.28	7	1
1:A:59:ASP:CB	1:A:62:ILE:HD11	0.62	2.25	19	8
1:A:133:HIS:CE1	1:B:137:ALA:HB1	0.62	2.29	18	4
1:B:95:THR:HG23	1:B:109:PRO:CB	0.62	2.23	12	1
1:A:61:MET:H	1:A:66:ILE:HD11	0.62	1.52	1	9
1:A:87:ILE:HD11	1:A:94:PHE:CD2	0.62	2.29	5	1
1:A:63:ASP:OD2	1:A:108:ILE:HD11	0.62	1.95	11	1
1:B:72:LEU:N	1:B:72:LEU:HD23	0.62	2.10	11	1
1:A:40:LEU:CG	1:A:44:LEU:HD22	0.62	2.25	18	1
1:B:105:VAL:O	1:B:105:VAL:HG13	0.62	1.92	14	3
1:A:59:ASP:HB2	1:A:62:ILE:HD11	0.62	1.71	16	8
1:A:87:ILE:HD11	1:A:94:PHE:CE2	0.62	2.30	5	1
1:B:97:LYS:CG	1:B:108:ILE:HG23	0.62	2.25	15	1
1:B:59:ASP:HB2	1:B:62:ILE:HD11	0.61	1.71	16	8
1:B:85:ILE:HG23	1:B:85:ILE:O	0.61	1.95	7	1
1:B:97:LYS:HG2	1:B:108:ILE:HG23	0.61	1.72	15	1
1:B:59:ASP:CB	1:B:62:ILE:HD11	0.61	2.25	4	7
1:A:105:VAL:HG23	1:A:105:VAL:O	0.61	1.95	15	14
1:A:41:ASN:CB	1:B:40:LEU:HD21	0.61	2.25	13	2
1:A:71:LEU:HD11	1:B:43:LEU:HD22	0.61	1.73	20	4
1:A:133:HIS:CD2	1:B:137:ALA:HB1	0.61	2.31	5	1
1:A:71:LEU:HD13	1:A:71:LEU:C	0.61	2.21	19	1
1:B:105:VAL:O	1:B:105:VAL:HG23	0.61	1.96	20	15
1:B:82:HIS:CE1	1:B:101:LEU:HD11	0.61	2.31	9	1
1:B:99:LEU:HD21	1:B:127:VAL:HG22	0.61	1.72	13	1
1:A:137:ALA:HB1	1:B:133:HIS:CE1	0.61	2.31	18	4
1:A:105:VAL:HG21	1:A:122:GLU:HA	0.61	1.73	10	1
1:A:64:GLY:O	1:A:132:ILE:HG21	0.61	1.96	3	3
1:A:124:THR:O	1:A:125:LEU:HD22	0.61	1.96	17	14
1:A:85:ILE:HD11	1:A:96:VAL:CG1	0.60	2.26	3	1
1:A:71:LEU:HD22	1:A:72:LEU:N	0.60	2.11	5	6
1:B:71:LEU:HD22	1:B:72:LEU:N	0.60	2.11	5	6
1:B:101:LEU:HD23	1:B:125:LEU:HB3	0.60	1.72	9	1
1:B:88:ALA:CB	1:B:107:LEU:HD11	0.60	2.26	14	1
1:A:40:LEU:HD21	1:B:41:ASN:CB	0.60	2.25	13	2
1:A:40:LEU:HG	1:A:43:LEU:HD12	0.60	1.72	11	1
1:B:63:ASP:CG	1:B:108:ILE:HD11	0.60	2.21	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ILE:HD13	1:A:115:SER:C	0.60	2.21	2	6
1:A:43:LEU:HD11	1:A:44:LEU:CD1	0.60	2.27	5	5
1:B:72:LEU:HD21	1:B:132:ILE:HG23	0.60	1.72	16	4
1:B:108:ILE:HD13	1:B:110:MET:N	0.60	2.11	14	1
1:A:43:LEU:HD22	1:B:71:LEU:HD11	0.60	1.73	20	4
1:A:72:LEU:HD21	1:A:132:ILE:HG23	0.60	1.73	16	4
1:B:64:GLY:C	1:B:96:VAL:HG11	0.60	2.22	19	2
1:B:99:LEU:HD22	1:B:127:VAL:CG2	0.60	2.27	9	1
1:B:72:LEU:HD23	1:B:72:LEU:C	0.60	2.21	7	11
1:B:43:LEU:HD11	1:B:44:LEU:CD1	0.60	2.26	5	5
1:B:40:LEU:HG	1:B:43:LEU:HD12	0.60	1.73	11	1
1:B:43:LEU:CD2	1:B:44:LEU:HD13	0.60	2.26	13	1
1:B:64:GLY:O	1:B:132:ILE:HG21	0.60	1.96	3	2
1:B:130:VAL:HG22	1:B:130:VAL:O	0.60	1.97	13	17
1:B:124:THR:O	1:B:125:LEU:HD22	0.60	1.96	17	14
1:B:101:LEU:C	1:B:101:LEU:HD12	0.60	2.22	9	1
1:A:38:ILE:O	1:A:38:ILE:HG23	0.59	1.96	13	8
1:B:132:ILE:O	1:B:132:ILE:HG22	0.59	1.97	3	15
1:A:43:LEU:CD2	1:A:44:LEU:HD13	0.59	2.26	13	1
1:B:101:LEU:HD13	1:B:125:LEU:HB3	0.59	1.72	13	2
1:A:108:ILE:O	1:A:108:ILE:HG23	0.59	1.97	7	2
1:A:105:VAL:HG21	1:A:120:SER:O	0.59	1.97	1	4
1:A:72:LEU:HD23	1:A:72:LEU:C	0.59	2.21	7	11
1:A:73:ILE:HD11	1:B:43:LEU:HD13	0.59	1.74	15	6
1:B:38:ILE:HG23	1:B:38:ILE:O	0.59	1.97	20	5
1:A:137:ALA:HB1	1:B:133:HIS:CD2	0.59	2.33	5	1
1:B:40:LEU:CG	1:B:44:LEU:HD22	0.59	2.26	18	1
1:A:95:THR:HG23	1:A:109:PRO:HB3	0.59	1.74	19	1
1:A:90:VAL:HG23	1:A:124:THR:O	0.59	1.98	4	13
1:B:63:ASP:HB2	1:B:110:MET:HE2	0.59	1.73	8	2
1:A:108:ILE:HD13	1:A:108:ILE:O	0.59	1.97	1	2
1:A:132:ILE:HG22	1:A:132:ILE:O	0.59	1.97	3	16
1:B:45:ILE:HG21	1:B:51:THR:HG21	0.59	1.73	7	3
1:A:65:GLY:C	1:A:72:LEU:HD23	0.59	2.23	20	1
1:B:90:VAL:HG23	1:B:124:THR:O	0.59	1.97	4	13
1:A:130:VAL:HG22	1:A:130:VAL:O	0.59	1.97	13	17
1:B:96:VAL:H	1:B:108:ILE:HD12	0.59	1.56	16	1
1:A:45:ILE:HG21	1:A:51:THR:HG21	0.59	1.73	7	3
1:A:45:ILE:CG2	1:A:51:THR:HG21	0.59	2.27	7	2
1:A:40:LEU:HD13	1:B:45:ILE:HG13	0.58	1.73	9	1
1:B:131:VAL:O	1:B:132:ILE:HD12	0.58	1.98	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:LEU:HD13	1:B:132:ILE:HG23	0.58	1.74	3	1
1:B:65:GLY:C	1:B:72:LEU:HD23	0.58	2.23	20	1
1:A:54:VAL:CG1	1:A:72:LEU:HD23	0.58	2.28	3	1
1:B:45:ILE:CG2	1:B:51:THR:HG21	0.58	2.28	7	2
1:A:45:ILE:HG13	1:B:40:LEU:HD13	0.58	1.74	9	1
1:A:72:LEU:HD13	1:A:132:ILE:HG23	0.58	1.74	3	1
1:A:131:VAL:O	1:A:132:ILE:HD12	0.58	1.98	8	3
1:B:64:GLY:HA2	1:B:96:VAL:HG11	0.58	1.74	18	1
1:B:99:LEU:HD23	1:B:99:LEU:H	0.58	1.59	13	14
1:A:40:LEU:HG	1:A:44:LEU:HD22	0.58	1.76	18	1
1:A:75:ASP:CB	1:A:131:VAL:HG12	0.58	2.28	3	4
1:B:54:VAL:CG1	1:B:72:LEU:HD23	0.58	2.28	3	1
1:A:99:LEU:H	1:A:99:LEU:HD23	0.58	1.59	2	13
1:A:87:ILE:O	1:A:87:ILE:HG23	0.57	1.98	16	18
1:A:74:VAL:HG23	1:A:131:VAL:O	0.57	1.99	12	8
1:A:108:ILE:HD11	1:A:115:SER:N	0.57	2.13	15	5
1:A:40:LEU:HD22	1:B:45:ILE:HD12	0.57	1.76	6	1
1:A:131:VAL:HG21	1:A:133:HIS:CE1	0.57	2.35	7	6
1:A:135:VAL:CG2	1:B:135:VAL:HG22	0.57	2.27	3	1
1:A:108:ILE:HG23	1:A:108:ILE:O	0.57	1.98	19	8
1:A:40:LEU:HA	1:A:43:LEU:HD23	0.57	1.77	8	4
1:A:105:VAL:HG22	1:A:119:ILE:HB	0.57	1.77	20	2
1:A:71:LEU:HD11	1:B:44:LEU:HD11	0.57	1.76	18	5
1:B:40:LEU:HA	1:B:43:LEU:HD23	0.57	1.77	8	4
1:A:43:LEU:HD13	1:B:73:ILE:HD11	0.57	1.74	15	6
1:B:59:ASP:HA	1:B:62:ILE:HD11	0.57	1.76	3	5
1:B:74:VAL:HG23	1:B:131:VAL:O	0.57	1.99	12	8
1:A:38:ILE:HG23	1:B:53:PHE:HE2	0.57	1.59	6	1
1:A:72:LEU:HD13	1:A:72:LEU:C	0.57	2.24	17	3
1:A:108:ILE:HD13	1:A:108:ILE:C	0.57	2.24	18	1
1:B:82:HIS:NE2	1:B:101:LEU:HD11	0.57	2.15	9	1
1:B:108:ILE:HD13	1:B:108:ILE:C	0.56	2.24	1	1
1:B:75:ASP:CB	1:B:131:VAL:HG12	0.56	2.29	3	3
1:B:131:VAL:HG21	1:B:133:HIS:CE1	0.56	2.35	7	6
1:A:45:ILE:HD12	1:B:40:LEU:HG	0.56	1.76	20	2
1:B:107:LEU:HD13	1:B:119:ILE:CD1	0.56	2.15	11	2
1:B:101:LEU:HD12	1:B:102:ARG:N	0.56	2.15	9	1
1:A:99:LEU:HD13	1:A:107:LEU:CD1	0.56	2.30	16	3
1:B:87:ILE:HG23	1:B:87:ILE:O	0.56	1.98	16	16
1:B:72:LEU:HD13	1:B:72:LEU:C	0.56	2.24	17	4
1:A:40:LEU:HG	1:B:45:ILE:HD12	0.56	1.77	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:LEU:HB2	1:A:119:ILE:HD11	0.56	1.77	13	3
1:A:59:ASP:HA	1:A:62:ILE:HD11	0.56	1.76	3	6
1:A:45:ILE:HD12	1:B:40:LEU:HD22	0.56	1.75	6	1
1:A:62:ILE:HD12	1:A:111:ASN:CB	0.56	2.30	7	1
1:B:99:LEU:HD13	1:B:107:LEU:CD1	0.56	2.31	15	5
1:B:108:ILE:HD13	1:B:115:SER:C	0.56	2.25	2	6
1:A:117:ILE:HG23	1:A:117:ILE:O	0.56	2.00	7	1
1:B:52:TYR:HB2	1:B:74:VAL:HG13	0.56	1.77	20	1
1:B:95:THR:HG21	1:B:107:LEU:HD21	0.56	1.77	4	2
1:B:117:ILE:HG23	1:B:117:ILE:O	0.56	2.00	14	5
1:B:40:LEU:HG	1:B:44:LEU:HD22	0.56	1.77	18	1
1:A:100:GLN:C	1:A:101:LEU:HD23	0.56	2.25	20	8
1:A:44:LEU:HD11	1:B:71:LEU:HD11	0.56	1.76	18	5
1:B:88:ALA:HB3	1:B:95:THR:HG1	0.56	1.61	19	2
1:B:72:LEU:HD12	1:B:72:LEU:C	0.55	2.26	3	1
1:A:45:ILE:HG12	1:A:51:THR:HG21	0.55	1.78	19	1
1:A:78:ILE:HD13	1:A:130:VAL:HG11	0.55	1.77	13	1
1:B:105:VAL:HG11	1:B:119:ILE:O	0.55	2.01	14	1
1:B:45:ILE:HG12	1:B:51:THR:HG21	0.55	1.78	19	1
1:A:52:TYR:HB2	1:A:74:VAL:HG13	0.55	1.77	20	1
1:A:72:LEU:HD12	1:A:72:LEU:C	0.55	2.26	3	1
1:B:78:ILE:HD13	1:B:130:VAL:HG11	0.55	1.78	13	1
1:B:80:ALA:HB1	1:B:86:VAL:CG1	0.55	2.32	15	6
1:A:45:ILE:CD1	1:B:40:LEU:HD11	0.55	2.25	7	2
1:A:43:LEU:HD12	1:A:43:LEU:N	0.55	2.17	10	2
1:B:65:GLY:O	1:B:72:LEU:HD12	0.55	2.02	19	2
1:B:100:GLN:C	1:B:101:LEU:HD23	0.55	2.26	16	12
1:B:38:ILE:H	1:B:38:ILE:HD13	0.55	1.61	9	1
1:A:101:LEU:HD13	1:A:125:LEU:HB3	0.55	1.77	13	2
1:B:108:ILE:O	1:B:108:ILE:HG23	0.55	2.02	8	2
1:B:43:LEU:HD12	1:B:43:LEU:N	0.55	2.17	10	2
1:B:105:VAL:HG11	1:B:122:GLU:H	0.55	1.62	17	4
1:B:62:ILE:HD12	1:B:111:ASN:CB	0.54	2.32	7	2
1:A:40:LEU:HD12	1:B:45:ILE:CD1	0.54	2.28	2	1
1:A:38:ILE:CG1	1:A:40:LEU:HD23	0.54	2.32	1	1
1:A:80:ALA:HB1	1:A:86:VAL:CG1	0.54	2.32	15	4
1:A:82:HIS:CE1	1:A:101:LEU:CD1	0.54	2.91	7	1
1:A:96:VAL:H	1:A:108:ILE:HD12	0.54	1.61	11	2
1:A:135:VAL:HG22	1:B:135:VAL:CG2	0.54	2.27	3	1
1:B:102:ARG:HB2	1:B:103:PRO:HD3	0.54	1.80	8	2
1:B:105:VAL:HG11	1:B:122:GLU:CB	0.54	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD12	1:A:101:LEU:C	0.54	2.27	7	1
1:B:82:HIS:CE1	1:B:101:LEU:CD1	0.54	2.90	9	1
1:A:65:GLY:O	1:A:72:LEU:HD12	0.54	2.03	19	2
1:B:43:LEU:CD1	1:B:44:LEU:CD1	0.54	2.86	7	5
1:B:72:LEU:HD11	1:B:131:VAL:CG2	0.54	2.33	20	1
1:B:99:LEU:CD1	1:B:101:LEU:HD11	0.54	2.32	14	3
1:B:45:ILE:HD12	1:B:51:THR:HG21	0.54	1.78	15	1
1:A:47:HIS:CD2	1:A:47:HIS:N	0.54	2.76	17	1
1:A:110:MET:HE3	1:A:110:MET:HA	0.54	1.80	20	1
1:B:54:VAL:HG12	1:B:72:LEU:HG	0.53	1.80	3	1
1:B:95:THR:HG21	1:B:107:LEU:CD1	0.53	2.25	5	1
1:B:61:MET:CG	1:B:96:VAL:HG21	0.53	2.33	7	1
1:B:106:GLN:C	1:B:107:LEU:HD12	0.53	2.26	7	1
1:B:96:VAL:N	1:B:108:ILE:HD12	0.53	2.18	16	1
1:B:105:VAL:HG11	1:B:122:GLU:CA	0.53	2.32	20	2
1:B:99:LEU:HD21	1:B:127:VAL:CG2	0.53	2.34	13	1
1:A:56:ALA:HB1	1:A:66:ILE:CA	0.53	2.34	18	8
1:B:108:ILE:HD11	1:B:115:SER:N	0.53	2.19	5	3
1:A:43:LEU:CD1	1:A:44:LEU:CD1	0.53	2.86	7	5
1:B:105:VAL:HG11	1:B:122:GLU:HB2	0.53	1.80	5	2
1:A:43:LEU:CD1	1:B:53:PHE:CD2	0.53	2.92	19	1
1:A:119:ILE:HG21	1:A:125:LEU:HD21	0.53	1.80	1	1
1:B:134:VAL:O	1:B:134:VAL:HG23	0.53	2.03	19	3
1:B:56:ALA:HB1	1:B:66:ILE:CA	0.53	2.34	18	8
1:A:71:LEU:HD11	1:A:73:ILE:CD1	0.53	2.33	3	2
1:B:105:VAL:HG23	1:B:118:THR:OG1	0.53	2.02	16	2
1:A:40:LEU:C	1:A:40:LEU:HD13	0.53	2.29	10	1
1:A:72:LEU:HD11	1:A:131:VAL:CG2	0.53	2.33	20	1
1:A:134:VAL:HG23	1:A:134:VAL:O	0.53	2.03	19	3
1:B:71:LEU:HD11	1:B:73:ILE:CD1	0.53	2.33	3	2
1:A:85:ILE:HG22	1:B:139:ARG:C	0.53	2.29	7	4
1:B:132:ILE:HG22	1:B:132:ILE:O	0.53	2.02	7	1
1:A:102:ARG:CB	1:A:103:PRO:HD3	0.53	2.34	11	19
1:A:133:HIS:NE2	1:B:135:VAL:HG12	0.53	2.19	2	1
1:B:40:LEU:C	1:B:40:LEU:HD13	0.53	2.29	10	1
1:B:74:VAL:O	1:B:74:VAL:HG13	0.53	2.04	17	1
1:A:73:ILE:CD1	1:B:44:LEU:HD21	0.53	2.34	7	1
1:B:99:LEU:H	1:B:99:LEU:HD23	0.53	1.63	7	1
1:A:119:ILE:HG21	1:A:125:LEU:HD23	0.53	1.80	11	2
1:A:45:ILE:HD12	1:A:51:THR:HG21	0.53	1.78	15	1
1:A:74:VAL:HG13	1:A:74:VAL:O	0.53	2.04	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:PHE:CD2	1:B:43:LEU:CD1	0.53	2.92	19	1
1:A:66:ILE:O	1:A:66:ILE:HD12	0.53	2.04	7	1
1:A:40:LEU:HA	1:A:43:LEU:HD11	0.53	1.81	10	2
1:A:54:VAL:HG12	1:A:72:LEU:HG	0.52	1.80	3	1
1:A:44:LEU:HD21	1:B:73:ILE:CD1	0.52	2.34	7	1
1:B:90:VAL:HG21	1:B:125:LEU:HD21	0.52	1.79	8	1
1:B:105:VAL:HG11	1:B:122:GLU:N	0.52	2.18	15	5
1:A:97:LYS:HD2	1:A:108:ILE:HG23	0.52	1.81	6	2
1:A:139:ARG:C	1:B:85:ILE:HG22	0.52	2.29	7	3
1:A:105:VAL:HG21	1:A:122:GLU:CA	0.52	2.33	10	1
1:A:52:TYR:CB	1:A:74:VAL:HG13	0.52	2.35	20	8
1:B:87:ILE:O	1:B:87:ILE:HG23	0.52	2.03	15	2
1:B:102:ARG:CB	1:B:103:PRO:HD3	0.52	2.35	11	19
1:A:40:LEU:HD11	1:B:45:ILE:CD1	0.52	2.25	7	2
1:B:105:VAL:HG21	1:B:119:ILE:O	0.52	2.04	9	1
1:A:62:ILE:HG23	1:A:67:SER:HG	0.52	1.64	16	1
1:A:97:LYS:HG2	1:A:108:ILE:HG23	0.52	1.82	16	2
1:B:40:LEU:HD13	1:B:40:LEU:O	0.52	2.05	10	1
1:A:102:ARG:N	1:A:103:PRO:CD	0.52	2.72	13	1
1:B:71:LEU:HD13	1:B:71:LEU:O	0.52	2.05	15	1
1:A:114:TYR:O	1:A:114:TYR:CD2	0.52	2.63	13	15
1:B:40:LEU:HA	1:B:43:LEU:HD11	0.52	1.80	10	2
1:A:63:ASP:HB2	1:A:110:MET:HE3	0.52	1.82	14	1
1:A:102:ARG:CB	1:A:103:PRO:CD	0.52	2.87	11	19
1:A:73:ILE:HD11	1:B:43:LEU:HD11	0.52	1.81	4	2
1:B:63:ASP:O	1:B:85:ILE:HD11	0.52	2.05	20	1
1:A:135:VAL:HG12	1:B:133:HIS:NE2	0.52	2.19	2	1
1:A:63:ASP:O	1:A:85:ILE:HD11	0.52	2.05	20	1
1:A:90:VAL:HG21	1:A:125:LEU:HD21	0.51	1.80	8	1
1:A:101:LEU:HD11	1:A:125:LEU:HB3	0.51	1.82	11	2
1:B:38:ILE:O	1:B:38:ILE:HG23	0.51	2.04	7	1
1:B:47:HIS:CD2	1:B:47:HIS:N	0.51	2.76	17	1
1:B:85:ILE:O	1:B:85:ILE:CG2	0.51	2.59	11	11
1:B:38:ILE:HD13	1:B:38:ILE:N	0.51	2.20	9	1
1:B:101:LEU:HD11	1:B:125:LEU:HB3	0.51	1.81	11	1
1:A:85:ILE:O	1:A:85:ILE:CG2	0.51	2.59	11	7
1:B:119:ILE:HG21	1:B:125:LEU:HD23	0.51	1.83	11	4
1:B:52:TYR:CB	1:B:74:VAL:HG13	0.51	2.35	20	7
1:B:102:ARG:CB	1:B:103:PRO:CD	0.51	2.89	11	18
1:B:108:ILE:HD13	1:B:116:PRO:N	0.51	2.21	2	1
1:A:40:LEU:HD11	1:A:44:LEU:HD22	0.51	1.81	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ARG:HB2	1:A:103:PRO:HD3	0.51	1.81	10	2
1:B:114:TYR:CD2	1:B:114:TYR:O	0.51	2.64	14	13
1:B:105:VAL:HG12	1:B:119:ILE:HB	0.51	1.83	7	1
1:B:86:VAL:HG21	1:B:127:VAL:HG21	0.51	1.83	11	3
1:B:102:ARG:N	1:B:103:PRO:CD	0.51	2.74	14	3
1:B:109:PRO:O	1:B:110:MET:CB	0.51	2.58	11	11
1:A:43:LEU:HD11	1:B:73:ILE:CD1	0.51	2.36	12	3
1:B:90:VAL:CB	1:B:125:LEU:HD22	0.51	2.36	5	3
1:A:95:THR:HG23	1:A:109:PRO:CB	0.51	2.35	19	1
1:A:102:ARG:HB2	1:A:103:PRO:CD	0.50	2.36	10	1
1:B:85:ILE:HG21	1:B:132:ILE:HD12	0.50	1.83	20	1
1:B:94:PHE:O	1:B:95:THR:HG23	0.50	2.06	1	1
1:A:85:ILE:HD13	1:A:85:ILE:O	0.50	2.06	3	2
1:A:73:ILE:CD1	1:B:43:LEU:HD11	0.50	2.36	12	3
1:A:105:VAL:HG11	1:A:122:GLU:CB	0.50	2.37	5	1
1:A:62:ILE:HD12	1:A:111:ASN:HB2	0.50	1.83	7	1
1:A:39:ASP:O	1:A:41:ASN:N	0.50	2.45	2	1
1:A:43:LEU:HD11	1:B:73:ILE:HD11	0.50	1.82	4	2
1:A:107:LEU:HG	1:A:108:ILE:HG22	0.50	1.84	13	1
1:A:45:ILE:HD12	1:B:40:LEU:HD21	0.50	1.84	16	2
1:A:52:TYR:HB3	1:A:74:VAL:HG13	0.50	1.83	17	1
1:B:52:TYR:HB3	1:B:74:VAL:HG13	0.50	1.83	17	1
1:A:119:ILE:HG21	1:A:125:LEU:CD2	0.50	2.37	1	3
1:A:117:ILE:O	1:A:117:ILE:HG23	0.50	2.07	17	5
1:A:71:LEU:HD11	1:B:44:LEU:CD1	0.50	2.36	6	5
1:A:139:ARG:CB	1:B:131:VAL:HG23	0.50	2.37	5	1
1:A:40:LEU:HD13	1:A:40:LEU:O	0.50	2.05	10	1
1:B:39:ASP:O	1:B:41:ASN:N	0.50	2.45	2	1
1:B:118:THR:HG23	1:B:118:THR:O	0.50	2.06	7	1
1:B:87:ILE:HG22	1:B:129:GLY:O	0.50	2.07	20	1
1:A:90:VAL:CB	1:A:125:LEU:HD22	0.50	2.36	5	3
1:B:43:LEU:HG	1:B:44:LEU:HD13	0.50	1.84	7	4
1:A:71:LEU:HD13	1:A:71:LEU:O	0.50	2.05	15	1
1:A:85:ILE:HG21	1:A:132:ILE:HD12	0.50	1.82	20	1
1:A:63:ASP:HB2	1:A:110:MET:HE2	0.50	1.84	1	2
1:A:72:LEU:N	1:A:72:LEU:CD2	0.50	2.74	11	1
1:A:137:ALA:CB	1:B:133:HIS:CE1	0.50	2.94	11	2
1:A:87:ILE:HG22	1:A:129:GLY:O	0.50	2.07	20	1
1:A:44:LEU:HD23	1:B:44:LEU:CB	0.49	2.37	13	6
1:A:45:ILE:CD1	1:B:40:LEU:HD12	0.49	2.28	2	1
1:B:80:ALA:HA	1:B:130:VAL:HG23	0.49	1.84	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD11	1:B:135:VAL:HG21	0.49	1.83	11	1
1:A:133:HIS:CE1	1:B:137:ALA:CB	0.49	2.95	11	2
1:A:72:LEU:HD21	1:A:132:ILE:HG22	0.49	1.84	17	1
1:B:114:TYR:O	1:B:114:TYR:CD1	0.49	2.65	4	1
1:A:44:LEU:CD1	1:B:71:LEU:HD11	0.49	2.36	6	5
1:A:137:ALA:CB	1:B:133:HIS:CD2	0.49	2.95	8	4
1:B:107:LEU:HD21	1:B:125:LEU:HD12	0.49	1.84	7	1
1:B:61:MET:HE2	1:B:109:PRO:CB	0.49	2.37	12	1
1:A:41:ASN:HB2	1:B:40:LEU:HD21	0.49	1.84	13	1
1:A:86:VAL:HG21	1:A:127:VAL:HG21	0.49	1.83	11	2
1:B:85:ILE:HD13	1:B:85:ILE:O	0.49	2.08	3	2
1:A:63:ASP:OD1	1:A:64:GLY:N	0.49	2.44	5	17
1:A:44:LEU:CB	1:B:44:LEU:HD23	0.49	2.37	13	6
1:A:133:HIS:CD2	1:B:137:ALA:CB	0.49	2.95	8	4
1:A:72:LEU:C	1:A:72:LEU:HD13	0.49	2.33	2	1
1:A:82:HIS:CE1	1:A:101:LEU:CG	0.49	2.95	7	1
1:B:107:LEU:CD1	1:B:119:ILE:HD11	0.49	2.18	11	1
1:B:102:ARG:HB2	1:B:103:PRO:CD	0.49	2.36	8	1
1:A:85:ILE:HD13	1:B:138:MET:CG	0.49	2.38	14	1
1:A:114:TYR:CD1	1:A:114:TYR:O	0.49	2.66	17	3
1:A:131:VAL:HG23	1:B:139:ARG:CB	0.49	2.37	5	1
1:B:40:LEU:HD12	1:B:44:LEU:HD22	0.49	1.81	8	1
1:A:97:LYS:N	1:A:97:LYS:CE	0.49	2.75	20	1
1:A:43:LEU:HG	1:A:44:LEU:HD13	0.49	1.84	7	4
1:A:50:ALA:HB1	1:A:77:ALA:CB	0.49	2.36	12	2
1:A:137:ALA:N	1:B:133:HIS:CD2	0.49	2.81	2	1
1:B:50:ALA:HB1	1:B:77:ALA:CB	0.49	2.36	12	2
1:B:46:GLN:C	1:B:47:HIS:CG	0.48	2.92	10	5
1:A:80:ALA:HA	1:A:130:VAL:HG23	0.48	1.85	4	3
1:A:56:ALA:HB1	1:A:66:ILE:HA	0.48	1.85	18	2
1:A:54:VAL:CG1	1:A:72:LEU:CD1	0.48	2.91	11	1
1:A:107:LEU:HB3	1:A:117:ILE:HG23	0.48	1.83	13	1
1:B:117:ILE:HD13	1:B:118:THR:N	0.48	2.23	15	1
1:B:119:ILE:HG22	1:B:120:SER:N	0.48	2.23	7	14
1:A:82:HIS:CE1	1:A:101:LEU:HG	0.48	2.43	7	1
1:B:108:ILE:O	1:B:108:ILE:CG2	0.48	2.61	14	3
1:B:43:LEU:HD12	1:B:44:LEU:N	0.48	2.23	9	2
1:A:131:VAL:HG23	1:B:139:ARG:HB2	0.48	1.84	18	4
1:A:45:ILE:CD1	1:B:40:LEU:CD1	0.48	2.91	19	2
1:B:72:LEU:N	1:B:72:LEU:CD2	0.48	2.75	11	1
1:A:40:LEU:HD21	1:B:41:ASN:HB2	0.48	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD11	1:B:53:PHE:CB	0.48	2.38	15	1
1:B:72:LEU:HD21	1:B:132:ILE:HG22	0.48	1.85	17	1
1:A:133:HIS:CD2	1:B:137:ALA:N	0.48	2.81	2	1
1:A:46:GLN:C	1:A:47:HIS:CG	0.48	2.91	9	5
1:A:38:ILE:HG23	1:B:53:PHE:CE2	0.48	2.42	6	1
1:B:114:TYR:CD1	1:B:114:TYR:N	0.48	2.82	8	3
1:B:62:ILE:HG23	1:B:67:SER:HG	0.48	1.68	16	1
1:A:45:ILE:HG22	1:A:46:GLN:N	0.48	2.24	13	6
1:A:86:VAL:HG21	1:A:127:VAL:CG2	0.48	2.38	9	3
1:B:56:ALA:HB1	1:B:66:ILE:HA	0.48	1.85	18	2
1:A:40:LEU:HD12	1:A:40:LEU:C	0.48	2.33	15	1
1:A:85:ILE:C	1:A:85:ILE:CD1	0.48	2.86	15	4
1:B:75:ASP:CB	1:B:131:VAL:CG1	0.48	2.92	3	2
1:B:119:ILE:HG21	1:B:125:LEU:CD2	0.48	2.39	9	2
1:A:88:ALA:HB3	1:A:95:THR:HG1	0.48	1.67	11	2
1:A:40:LEU:HD21	1:B:45:ILE:HD12	0.48	1.84	16	2
1:B:73:ILE:O	1:B:131:VAL:HG13	0.48	2.09	19	1
1:B:63:ASP:OD1	1:B:64:GLY:N	0.48	2.47	5	17
1:B:114:TYR:O	1:B:114:TYR:CG	0.48	2.67	11	9
1:A:52:TYR:CB	1:A:74:VAL:CG1	0.48	2.92	20	3
1:B:85:ILE:C	1:B:86:VAL:HG13	0.48	2.34	7	3
1:B:38:ILE:N	1:B:38:ILE:CD1	0.48	2.77	9	1
1:B:108:ILE:O	1:B:108:ILE:CD1	0.48	2.62	8	3
1:B:45:ILE:HG22	1:B:46:GLN:N	0.48	2.24	6	6
1:A:66:ILE:HD12	1:A:66:ILE:C	0.48	2.34	3	2
1:A:75:ASP:CB	1:A:131:VAL:CG1	0.48	2.92	3	2
1:B:85:ILE:C	1:B:85:ILE:CD1	0.48	2.86	11	4
1:B:54:VAL:CG1	1:B:72:LEU:CD1	0.48	2.91	11	1
1:A:45:ILE:HD12	1:B:40:LEU:CD2	0.48	2.39	16	1
1:A:95:THR:OG1	1:A:107:LEU:HD21	0.48	2.09	3	2
1:A:95:THR:HG21	1:A:107:LEU:HD21	0.48	1.85	6	3
1:A:40:LEU:C	1:A:40:LEU:CD1	0.48	2.87	9	2
1:A:43:LEU:HD12	1:A:44:LEU:N	0.48	2.24	9	2
1:A:95:THR:HG21	1:A:107:LEU:HG	0.48	1.86	19	1
1:A:44:LEU:CD1	1:B:71:LEU:CD1	0.47	2.91	16	8
1:A:71:LEU:CD1	1:B:44:LEU:CD1	0.47	2.91	16	7
1:A:73:ILE:CD1	1:B:43:LEU:CD1	0.47	2.92	4	5
1:B:119:ILE:HG21	1:B:125:LEU:HD21	0.47	1.84	1	1
1:A:71:LEU:HD21	1:B:43:LEU:HD21	0.47	1.85	4	1
1:A:71:LEU:HD22	1:A:71:LEU:C	0.47	2.34	5	2
1:B:43:LEU:CD1	1:B:44:LEU:N	0.47	2.77	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:99:LEU:HD22	1:B:127:VAL:HG22	0.47	1.85	9	1
1:B:84:ASP:N	1:B:98:LYS:CG	0.47	2.76	18	1
1:A:80:ALA:CB	1:A:86:VAL:CG1	0.47	2.92	14	5
1:B:52:TYR:CB	1:B:74:VAL:CG1	0.47	2.92	20	3
1:B:66:ILE:HD12	1:B:66:ILE:C	0.47	2.34	3	1
1:B:95:THR:HG21	1:B:107:LEU:HD12	0.47	1.85	8	1
1:A:40:LEU:CD1	1:A:44:LEU:HD21	0.47	2.39	14	1
1:B:40:LEU:CD1	1:B:44:LEU:HD21	0.47	2.39	14	1
1:A:139:ARG:HB2	1:B:131:VAL:HG23	0.47	1.85	18	2
1:B:67:SER:O	1:B:68:ASP:C	0.47	2.57	15	16
1:B:80:ALA:CB	1:B:86:VAL:CG1	0.47	2.92	14	4
1:A:105:VAL:O	1:A:105:VAL:CG1	0.47	2.63	7	3
1:B:86:VAL:HG21	1:B:127:VAL:CG2	0.47	2.39	9	3
1:A:43:LEU:CD1	1:A:44:LEU:N	0.47	2.78	10	2
1:B:46:GLN:O	1:B:47:HIS:CG	0.47	2.68	13	1
1:B:105:VAL:O	1:B:105:VAL:CG1	0.47	2.62	14	2
1:A:64:GLY:CA	1:A:96:VAL:CG1	0.47	2.91	18	1
1:A:73:ILE:O	1:A:131:VAL:HG13	0.47	2.09	19	1
1:A:78:ILE:HG22	1:A:79:THR:N	0.47	2.25	7	8
1:A:40:LEU:CD1	1:B:40:LEU:CD1	0.47	2.92	6	2
1:A:67:SER:O	1:A:68:ASP:C	0.47	2.57	15	16
1:A:108:ILE:CD1	1:A:115:SER:N	0.47	2.78	4	5
1:A:40:LEU:HD13	1:B:41:ASN:HB2	0.47	1.83	5	1
1:A:63:ASP:HB3	1:A:110:MET:HB2	0.47	1.87	5	2
1:A:137:ALA:CB	1:B:133:HIS:NE2	0.47	2.78	16	3
1:A:40:LEU:CD2	1:B:45:ILE:HD12	0.47	2.39	16	1
1:A:95:THR:HG21	1:A:107:LEU:CG	0.47	2.39	19	1
1:B:40:LEU:CD1	1:B:44:LEU:CD2	0.47	2.93	14	4
1:A:40:LEU:CD1	1:B:45:ILE:CD1	0.47	2.92	14	2
1:B:65:GLY:HA3	1:B:134:VAL:HG22	0.47	1.86	15	1
1:A:43:LEU:CD1	1:B:73:ILE:CD1	0.47	2.92	4	5
1:B:93:GLU:O	1:B:94:PHE:CG	0.47	2.68	1	1
1:A:109:PRO:O	1:A:110:MET:CB	0.47	2.61	11	9
1:A:93:GLU:O	1:A:94:PHE:CD1	0.47	2.68	19	3
1:B:114:TYR:CD2	1:B:115:SER:O	0.47	2.68	18	3
1:A:40:LEU:CD2	1:B:41:ASN:CB	0.47	2.92	13	1
1:B:78:ILE:HG22	1:B:79:THR:N	0.47	2.25	7	7
1:A:43:LEU:CD2	1:B:71:LEU:HD11	0.47	2.38	20	2
1:A:85:ILE:HD12	1:B:138:MET:HE2	0.47	1.86	2	1
1:A:85:ILE:C	1:A:86:VAL:HG13	0.47	2.35	9	3
1:A:136:LYS:C	1:B:133:HIS:CD2	0.47	2.93	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:VAL:CG1	1:A:72:LEU:CD2	0.47	2.93	3	1
1:A:133:HIS:NE2	1:B:137:ALA:CB	0.47	2.78	6	4
1:B:86:VAL:CG2	1:B:99:LEU:HD22	0.47	2.39	6	1
1:A:135:VAL:HG21	1:B:44:LEU:HD11	0.47	1.86	11	1
1:A:53:PHE:CB	1:B:43:LEU:HD11	0.47	2.39	15	1
1:A:114:TYR:CD2	1:A:115:SER:O	0.47	2.68	7	1
1:A:90:VAL:CG2	1:A:125:LEU:HD21	0.47	2.40	8	1
1:A:99:LEU:CB	1:A:107:LEU:CD1	0.47	2.92	8	2
1:A:99:LEU:N	1:A:99:LEU:HD23	0.47	2.25	11	3
1:A:86:VAL:CG2	1:A:127:VAL:HG11	0.47	2.40	11	1
1:A:62:ILE:CD1	1:A:111:ASN:ND2	0.47	2.78	12	1
1:A:114:TYR:O	1:A:114:TYR:CG	0.47	2.68	13	11
1:A:138:MET:HE2	1:B:85:ILE:HD12	0.47	1.87	2	1
1:A:87:ILE:CD1	1:A:94:PHE:CE2	0.47	2.97	5	1
1:A:40:LEU:CB	1:B:45:ILE:CD1	0.47	2.93	6	1
1:A:87:ILE:HD12	1:A:95:THR:O	0.47	2.10	11	2
1:B:108:ILE:CD1	1:B:115:SER:N	0.47	2.77	17	2
1:A:107:LEU:O	1:A:108:ILE:C	0.47	2.57	13	3
1:B:107:LEU:O	1:B:108:ILE:C	0.47	2.57	7	4
1:B:40:LEU:HD11	1:B:44:LEU:HD22	0.47	1.86	18	2
1:A:131:VAL:HG22	1:A:132:ILE:N	0.46	2.26	4	15
1:B:82:HIS:CE1	1:B:101:LEU:HG	0.46	2.45	9	1
1:A:46:GLN:O	1:A:47:HIS:CG	0.46	2.68	13	1
1:A:44:LEU:N	1:A:44:LEU:HD13	0.46	2.25	15	2
1:B:117:ILE:HD13	1:B:117:ILE:C	0.46	2.35	15	1
1:A:41:ASN:CA	1:B:40:LEU:HD22	0.46	2.37	18	1
1:A:40:LEU:CD1	1:A:44:LEU:CD2	0.46	2.93	14	4
1:B:108:ILE:C	1:B:108:ILE:CD1	0.46	2.88	18	3
1:B:86:VAL:CG2	1:B:127:VAL:HG11	0.46	2.40	11	1
1:B:64:GLY:O	1:B:134:VAL:HG21	0.46	2.10	12	1
1:A:41:ASN:CB	1:B:40:LEU:CD2	0.46	2.92	13	1
1:B:44:LEU:HD13	1:B:44:LEU:N	0.46	2.25	15	2
1:B:47:HIS:CD2	1:B:47:HIS:O	0.46	2.68	17	1
1:A:133:HIS:CD2	1:B:136:LYS:C	0.46	2.93	2	1
1:A:46:GLN:O	1:A:47:HIS:CD2	0.46	2.68	3	2
1:B:46:GLN:O	1:B:47:HIS:CD2	0.46	2.68	3	2
1:A:64:GLY:O	1:A:134:VAL:HG21	0.46	2.10	12	1
1:A:52:TYR:O	1:A:74:VAL:CG1	0.46	2.64	4	19
1:A:137:ALA:N	1:B:133:HIS:NE2	0.46	2.64	2	1
1:A:40:LEU:HD12	1:A:44:LEU:HD22	0.46	1.81	8	2
1:B:90:VAL:CG2	1:B:125:LEU:HD21	0.46	2.40	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:96:VAL:HG12	1:B:97:LYS:H	0.46	1.70	14	2
1:A:38:ILE:HG12	1:A:40:LEU:HD23	0.46	1.87	9	2
1:A:119:ILE:HG22	1:A:120:SER:N	0.46	2.25	17	17
1:B:54:VAL:CG1	1:B:72:LEU:CD2	0.46	2.93	3	1
1:A:86:VAL:HA	1:A:132:ILE:HD11	0.46	1.87	7	1
1:B:119:ILE:CG2	1:B:120:SER:N	0.46	2.79	14	2
1:B:108:ILE:HD13	1:B:109:PRO:C	0.46	2.35	11	1
1:B:59:ASP:C	1:B:62:ILE:HD11	0.46	2.36	20	2
1:A:131:VAL:CG2	1:A:133:HIS:CE1	0.46	2.99	3	4
1:B:43:LEU:CD1	1:B:43:LEU:C	0.46	2.86	11	1
1:A:65:GLY:HA3	1:A:134:VAL:HG22	0.46	1.85	15	1
1:B:131:VAL:HG22	1:B:132:ILE:N	0.46	2.26	6	15
1:A:105:VAL:HG12	1:A:119:ILE:HD13	0.46	1.86	3	2
1:A:108:ILE:HD11	1:A:114:TYR:C	0.46	2.36	4	1
1:B:62:ILE:HD12	1:B:111:ASN:HB2	0.46	1.87	7	1
1:A:133:HIS:NE2	1:B:137:ALA:N	0.46	2.64	2	1
1:B:93:GLU:O	1:B:94:PHE:CD1	0.46	2.69	12	2
1:B:95:THR:CG2	1:B:107:LEU:HD11	0.46	2.30	5	1
1:A:59:ASP:C	1:A:62:ILE:HD11	0.46	2.36	15	2
1:A:63:ASP:OD2	1:A:110:MET:N	0.46	2.49	20	2
1:A:72:LEU:CD2	1:A:132:ILE:HG23	0.46	2.41	16	1
1:A:135:VAL:CG1	1:B:135:VAL:HG22	0.46	2.39	18	1
1:A:75:ASP:O	1:A:129:GLY:CA	0.46	2.64	19	17
1:A:131:VAL:CG2	1:A:133:HIS:NE2	0.46	2.79	14	2
1:A:47:HIS:CD2	1:A:47:HIS:O	0.46	2.68	17	1
1:A:66:ILE:HG22	1:A:72:LEU:HB2	0.46	1.88	20	1
1:B:66:ILE:HG22	1:B:72:LEU:HB2	0.46	1.87	20	1
1:A:108:ILE:O	1:A:108:ILE:CD1	0.46	2.64	14	3
1:B:131:VAL:CG2	1:B:133:HIS:NE2	0.46	2.79	14	2
1:A:39:ASP:O	1:A:40:LEU:C	0.46	2.59	2	1
1:A:71:LEU:HD11	1:B:43:LEU:CD2	0.46	2.38	20	2
1:B:131:VAL:CG2	1:B:133:HIS:CE1	0.46	2.99	3	4
1:A:45:ILE:CD1	1:B:40:LEU:CB	0.46	2.94	6	1
1:A:43:LEU:CG	1:A:44:LEU:HD13	0.46	2.41	8	3
1:B:80:ALA:HB3	1:B:127:VAL:HG11	0.45	1.88	4	1
1:B:86:VAL:HA	1:B:132:ILE:HD11	0.45	1.87	7	1
1:B:118:THR:O	1:B:118:THR:HG23	0.45	2.10	14	1
1:B:72:LEU:CD2	1:B:132:ILE:HG23	0.45	2.41	16	1
1:B:75:ASP:O	1:B:129:GLY:CA	0.45	2.64	19	17
1:B:107:LEU:HB2	1:B:119:ILE:HD11	0.45	1.87	1	1
1:A:53:PHE:CZ	1:B:43:LEU:HD22	0.45	2.46	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:HD12	1:A:101:LEU:HD11	0.45	1.87	2	1
1:B:84:ASP:O	1:B:86:VAL:N	0.45	2.50	19	8
1:B:43:LEU:CG	1:B:44:LEU:HD13	0.45	2.41	7	4
1:A:86:VAL:HA	1:A:132:ILE:HD13	0.45	1.89	8	1
1:A:95:THR:HG21	1:A:107:LEU:CD2	0.45	2.41	11	3
1:B:132:ILE:CG1	1:B:132:ILE:O	0.45	2.64	20	1
1:B:63:ASP:OD1	1:B:63:ASP:N	0.45	2.49	20	3
1:A:53:PHE:HE2	1:B:38:ILE:HG23	0.45	1.71	18	1
1:B:66:ILE:O	1:B:66:ILE:CD1	0.45	2.64	18	17
1:B:39:ASP:O	1:B:40:LEU:C	0.45	2.58	2	1
1:A:41:ASN:HB2	1:B:40:LEU:HD13	0.45	1.84	5	1
1:A:47:HIS:CD2	1:A:51:THR:OG1	0.45	2.69	17	1
1:A:85:ILE:CD1	1:B:138:MET:HE2	0.45	2.41	2	1
1:A:43:LEU:C	1:A:43:LEU:CD2	0.45	2.86	3	5
1:B:62:ILE:HG23	1:B:67:SER:CB	0.45	2.41	3	1
1:A:40:LEU:HD13	1:A:43:LEU:HD12	0.45	1.88	14	1
1:B:52:TYR:O	1:B:74:VAL:CG1	0.45	2.65	19	18
1:A:66:ILE:O	1:A:66:ILE:CD1	0.45	2.65	18	13
1:A:138:MET:HE2	1:B:85:ILE:CD1	0.45	2.42	2	1
1:A:90:VAL:CG2	1:A:125:LEU:CD2	0.45	2.94	8	1
1:B:74:VAL:HA	1:B:131:VAL:HG23	0.45	1.89	20	1
1:B:71:LEU:C	1:B:71:LEU:CD1	0.45	2.90	3	11
1:B:99:LEU:HD23	1:B:99:LEU:N	0.45	2.27	7	10
1:A:61:MET:HE2	1:A:96:VAL:HG23	0.45	1.88	4	1
1:B:71:LEU:HD22	1:B:71:LEU:C	0.45	2.34	5	2
1:A:94:PHE:O	1:A:95:THR:HG23	0.45	2.12	7	1
1:A:64:GLY:O	1:A:96:VAL:CG1	0.45	2.64	19	2
1:B:47:HIS:CD2	1:B:51:THR:OG1	0.45	2.69	17	1
1:A:87:ILE:HD12	1:A:96:VAL:HG22	0.45	1.88	15	2
1:B:66:ILE:O	1:B:66:ILE:CG1	0.45	2.65	7	17
1:B:101:LEU:CD1	1:B:125:LEU:O	0.45	2.65	7	9
1:A:43:LEU:HD22	1:B:53:PHE:CZ	0.45	2.46	7	1
1:A:66:ILE:O	1:A:66:ILE:CG1	0.45	2.65	7	17
1:B:96:VAL:HG12	1:B:97:LYS:N	0.45	2.27	7	1
1:B:99:LEU:HD11	1:B:127:VAL:HG23	0.45	1.89	10	1
1:A:104:THR:HG22	1:A:105:VAL:N	0.45	2.27	15	2
1:A:108:ILE:C	1:A:108:ILE:CD1	0.44	2.90	14	2
1:A:85:ILE:O	1:A:85:ILE:CD1	0.44	2.66	8	3
1:A:43:LEU:HD21	1:B:71:LEU:HD21	0.44	1.89	4	1
1:B:99:LEU:CD2	1:B:127:VAL:CG2	0.44	2.94	9	1
1:B:106:GLN:CA	1:B:119:ILE:HD12	0.44	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:VAL:HA	1:A:131:VAL:HG23	0.44	1.89	20	1
1:A:40:LEU:CD1	1:A:41:ASN:N	0.44	2.75	3	2
1:B:95:THR:HG23	1:B:109:PRO:CG	0.44	2.41	5	1
1:A:73:ILE:HG13	1:B:44:LEU:HD21	0.44	1.89	9	1
1:B:40:LEU:C	1:B:40:LEU:CD1	0.44	2.87	9	2
1:B:62:ILE:CD1	1:B:111:ASN:ND2	0.44	2.79	12	1
1:A:82:HIS:CD2	1:A:102:ARG:HD3	0.44	2.47	16	1
1:A:132:ILE:CG1	1:A:132:ILE:O	0.44	2.64	20	1
1:A:110:MET:O	1:A:112:SER:N	0.44	2.50	11	1
1:B:40:LEU:CD1	1:B:41:ASN:N	0.44	2.79	6	2
1:A:82:HIS:NE2	1:A:101:LEU:CD1	0.44	2.78	7	1
1:A:108:ILE:O	1:A:108:ILE:CG2	0.44	2.66	7	1
1:B:52:TYR:O	1:B:74:VAL:N	0.44	2.50	19	5
1:A:71:LEU:C	1:A:71:LEU:CD1	0.44	2.90	3	8
1:A:52:TYR:O	1:A:74:VAL:N	0.44	2.50	19	6
1:A:41:ASN:O	1:A:45:ILE:HD12	0.44	2.12	10	1
1:A:61:MET:HE2	1:A:109:PRO:CB	0.44	2.42	12	1
1:A:73:ILE:HB	1:A:133:HIS:CB	0.44	2.43	20	1
1:B:73:ILE:HB	1:B:133:HIS:CB	0.44	2.43	20	1
1:A:101:LEU:CD1	1:A:125:LEU:O	0.44	2.65	2	8
1:B:90:VAL:CG2	1:B:125:LEU:CD2	0.44	2.95	8	1
1:B:110:MET:SD	1:B:113:ALA:HB3	0.44	2.53	9	1
1:B:108:ILE:C	1:B:108:ILE:HD12	0.44	2.38	10	1
1:B:117:ILE:C	1:B:117:ILE:CD1	0.44	2.90	15	1
1:A:71:LEU:HD12	1:B:44:LEU:HD12	0.44	1.90	17	1
1:A:40:LEU:HD22	1:B:41:ASN:CA	0.44	2.37	18	1
1:A:39:ASP:O	1:A:43:LEU:N	0.44	2.51	5	5
1:A:72:LEU:C	1:A:72:LEU:CD1	0.44	2.91	20	3
1:A:95:THR:OG1	1:A:109:PRO:CG	0.44	2.66	2	1
1:A:99:LEU:HD23	1:A:99:LEU:N	0.44	2.28	2	3
1:A:84:ASP:O	1:A:86:VAL:N	0.44	2.51	19	6
1:A:59:ASP:O	1:A:111:ASN:ND2	0.44	2.51	5	2
1:A:118:THR:O	1:A:118:THR:HG23	0.44	2.12	11	2
1:B:115:SER:HB3	1:B:116:PRO:HD2	0.44	1.90	7	2
1:B:41:ASN:O	1:B:45:ILE:CG1	0.44	2.66	10	1
1:A:40:LEU:HD13	1:A:43:LEU:CD1	0.44	2.42	14	1
1:B:110:MET:SD	1:B:114:TYR:CE2	0.44	3.11	16	1
1:B:62:ILE:CG1	1:B:111:ASN:OD1	0.44	2.66	8	2
1:B:96:VAL:O	1:B:97:LYS:CB	0.44	2.64	14	6
1:B:43:LEU:C	1:B:43:LEU:CD2	0.44	2.91	14	5
1:B:39:ASP:O	1:B:43:LEU:N	0.44	2.51	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:98:LYS:O	1:B:98:LYS:CG	0.44	2.65	11	2
1:B:78:ILE:CD1	1:B:130:VAL:HG11	0.44	2.43	13	1
1:A:138:MET:CG	1:B:85:ILE:HD13	0.44	2.43	14	1
1:A:108:ILE:CG1	1:A:108:ILE:O	0.44	2.66	16	1
1:A:132:ILE:O	1:A:132:ILE:HG12	0.44	2.11	20	1
1:B:132:ILE:O	1:B:132:ILE:HG12	0.44	2.11	20	1
1:A:120:SER:O	1:A:122:GLU:N	0.44	2.51	14	5
1:A:39:ASP:CG	1:A:42:GLN:CB	0.44	2.91	7	2
1:A:44:LEU:HD23	1:B:44:LEU:CG	0.44	2.43	13	3
1:A:99:LEU:CD1	1:A:101:LEU:HD11	0.44	2.43	12	2
1:B:56:ALA:HB3	1:B:70:ASP:O	0.44	2.13	13	1
1:A:59:ASP:O	1:A:62:ILE:HD11	0.44	2.13	15	2
1:A:88:ALA:HB3	1:A:95:THR:HG22	0.43	1.81	2	1
1:B:85:ILE:O	1:B:85:ILE:CD1	0.43	2.66	8	3
1:B:86:VAL:HA	1:B:132:ILE:HD13	0.43	1.89	8	1
1:B:82:HIS:CE1	1:B:101:LEU:CG	0.43	3.01	9	1
1:A:97:LYS:CG	1:A:107:LEU:HD12	0.43	2.43	14	1
1:B:64:GLY:CA	1:B:96:VAL:CG1	0.43	2.92	18	2
1:B:97:LYS:CB	1:B:109:PRO:HD2	0.43	2.43	19	1
1:A:105:VAL:O	1:A:105:VAL:CG2	0.43	2.67	15	8
1:A:80:ALA:HB3	1:A:127:VAL:HG11	0.43	1.88	4	1
1:A:73:ILE:HD12	1:B:43:LEU:HD11	0.43	1.90	17	1
1:A:62:ILE:CD1	1:A:111:ASN:OD1	0.43	2.67	1	1
1:B:64:GLY:O	1:B:134:VAL:CG1	0.43	2.66	1	1
1:B:90:VAL:CG2	1:B:124:THR:O	0.43	2.67	7	7
1:A:63:ASP:OD1	1:A:63:ASP:N	0.43	2.47	20	3
1:A:75:ASP:OD2	1:A:131:VAL:CG1	0.43	2.66	10	1
1:A:40:LEU:CD2	1:B:45:ILE:HD11	0.43	2.42	1	1
1:A:62:ILE:CG1	1:A:111:ASN:OD1	0.43	2.66	1	1
1:A:108:ILE:HD13	1:A:116:PRO:CA	0.43	2.44	2	1
1:B:61:MET:O	1:B:66:ILE:CG1	0.43	2.67	9	2
1:A:41:ASN:O	1:A:45:ILE:CG1	0.43	2.66	10	1
1:B:41:ASN:O	1:B:45:ILE:HD12	0.43	2.12	10	1
1:A:41:ASN:CA	1:B:40:LEU:HD21	0.43	2.43	13	1
1:A:111:ASN:ND2	1:A:111:ASN:C	0.43	2.76	19	1
1:B:60:SER:O	1:B:110:MET:CG	0.43	2.66	19	1
1:A:110:MET:N	1:A:110:MET:SD	0.43	2.92	20	1
1:B:43:LEU:C	1:B:43:LEU:CD1	0.43	2.89	3	1
1:A:72:LEU:C	1:A:72:LEU:CD2	0.43	2.92	19	5
1:B:117:ILE:CG2	1:B:117:ILE:O	0.43	2.66	15	1
1:A:88:ALA:HB3	1:A:95:THR:HB	0.43	1.89	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:ILE:N	1:A:132:ILE:CD1	0.43	2.77	19	1
1:B:109:PRO:C	1:B:110:MET:CG	0.43	2.92	10	3
1:A:62:ILE:HG23	1:A:67:SER:CB	0.43	2.43	3	1
1:A:97:LYS:CD	1:A:108:ILE:HG23	0.43	2.44	3	1
1:B:95:THR:CG2	1:B:109:PRO:CG	0.43	2.96	3	1
1:B:72:LEU:C	1:B:72:LEU:CD1	0.43	2.91	20	4
1:B:105:VAL:O	1:B:105:VAL:CG2	0.43	2.67	15	5
1:B:59:ASP:C	1:B:111:ASN:OD1	0.43	2.61	8	1
1:A:107:LEU:CD2	1:A:119:ILE:HD11	0.43	2.30	14	1
1:A:40:LEU:HD21	1:B:44:LEU:CB	0.43	2.44	18	1
1:B:75:ASP:CG	1:B:131:VAL:CG1	0.43	2.92	2	11
1:A:96:VAL:HG12	1:A:97:LYS:N	0.43	2.29	7	1
1:B:39:ASP:CG	1:B:42:GLN:CB	0.43	2.92	8	2
1:A:108:ILE:C	1:A:108:ILE:HD12	0.43	2.38	20	2
1:A:75:ASP:CG	1:A:131:VAL:CG1	0.43	2.92	2	11
1:B:85:ILE:O	1:B:132:ILE:CD1	0.43	2.67	7	2
1:B:104:THR:HG22	1:B:105:VAL:N	0.43	2.28	16	4
1:B:75:ASP:OD2	1:B:131:VAL:CG1	0.43	2.66	10	1
1:A:40:LEU:HD21	1:B:41:ASN:CA	0.43	2.42	13	1
1:A:82:HIS:CE1	1:A:101:LEU:HB2	0.43	2.49	12	7
1:B:56:ALA:CB	1:B:70:ASP:OD1	0.43	2.67	18	6
1:A:43:LEU:C	1:A:43:LEU:CD1	0.43	2.89	3	2
1:A:43:LEU:CD1	1:A:44:LEU:HD13	0.43	2.44	5	1
1:A:43:LEU:HG	1:A:44:LEU:N	0.43	2.29	6	1
1:A:44:LEU:HD21	1:B:73:ILE:HG13	0.43	1.89	9	1
1:B:45:ILE:CG2	1:B:51:THR:OG1	0.43	2.67	11	2
1:B:45:ILE:CG1	1:B:51:THR:HG21	0.43	2.44	19	1
1:A:45:ILE:HD11	1:B:40:LEU:CD2	0.42	2.42	1	1
1:B:62:ILE:CD1	1:B:111:ASN:OD1	0.42	2.67	1	2
1:B:63:ASP:CB	1:B:110:MET:HB2	0.42	2.44	1	1
1:A:44:LEU:HD12	1:B:135:VAL:HG21	0.42	1.90	2	1
1:A:107:LEU:HD21	1:A:109:PRO:HG3	0.42	1.89	2	1
1:A:90:VAL:CG2	1:A:124:THR:O	0.42	2.67	15	8
1:A:45:ILE:O	1:A:46:GLN:CG	0.42	2.67	8	6
1:A:105:VAL:HG11	1:A:122:GLU:CA	0.42	2.43	16	2
1:B:45:ILE:O	1:B:46:GLN:CG	0.42	2.67	5	6
1:A:44:LEU:CG	1:B:44:LEU:HD23	0.42	2.44	13	3
1:B:72:LEU:CD1	1:B:72:LEU:C	0.42	2.92	10	1
1:B:109:PRO:O	1:B:110:MET:CG	0.42	2.67	11	2
1:A:56:ALA:HB3	1:A:70:ASP:O	0.42	2.14	13	1
1:A:60:SER:O	1:A:111:ASN:N	0.42	2.52	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:HIS:CD2	1:B:137:ALA:HA	0.42	2.50	20	4
1:A:137:ALA:HA	1:B:133:HIS:CD2	0.42	2.49	20	4
1:B:82:HIS:CE1	1:B:101:LEU:HB2	0.42	2.49	18	7
1:A:132:ILE:O	1:A:132:ILE:CG2	0.42	2.67	8	3
1:B:71:LEU:CD1	1:B:73:ILE:CD1	0.42	2.97	3	1
1:B:120:SER:O	1:B:122:GLU:N	0.42	2.52	7	4
1:B:96:VAL:O	1:B:97:LYS:HB3	0.42	2.14	7	1
1:B:95:THR:OG1	1:B:107:LEU:HD21	0.42	2.14	12	1
1:A:45:ILE:CG2	1:A:46:GLN:N	0.42	2.82	13	1
1:A:84:ASP:O	1:A:86:VAL:HG13	0.42	2.14	20	1
1:A:135:VAL:HG21	1:B:44:LEU:HD12	0.42	1.91	2	1
1:A:61:MET:CB	1:A:66:ILE:HD11	0.42	2.44	4	1
1:A:109:PRO:C	1:A:110:MET:CG	0.42	2.91	9	4
1:B:38:ILE:O	1:B:38:ILE:CG1	0.42	2.67	4	3
1:A:102:ARG:HB3	1:A:103:PRO:HD3	0.42	1.91	9	1
1:B:82:HIS:NE2	1:B:101:LEU:CD1	0.42	2.83	9	1
1:A:40:LEU:O	1:A:43:LEU:CD1	0.42	2.67	13	2
1:B:117:ILE:O	1:B:117:ILE:HG23	0.42	2.13	15	2
1:B:40:LEU:HD13	1:B:43:LEU:CD1	0.42	2.44	14	1
1:B:56:ALA:HB2	1:B:66:ILE:HG22	0.42	1.91	14	1
1:A:40:LEU:HD21	1:B:44:LEU:HB2	0.42	1.92	18	1
1:A:97:LYS:NZ	1:A:107:LEU:HD11	0.42	2.29	20	1
1:B:45:ILE:HG22	1:B:46:GLN:H	0.42	1.74	20	1
1:B:86:VAL:HB	1:B:127:VAL:HG11	0.42	1.91	11	3
1:B:130:VAL:O	1:B:130:VAL:CG2	0.42	2.68	3	3
1:A:85:ILE:O	1:A:132:ILE:CD1	0.42	2.67	7	2
1:B:72:LEU:C	1:B:72:LEU:CD2	0.42	2.93	7	6
1:B:115:SER:CB	1:B:116:PRO:CD	0.42	2.97	7	2
1:B:84:ASP:C	1:B:98:LYS:CG	0.42	2.93	9	1
1:A:41:ASN:HB2	1:A:45:ILE:HD12	0.42	1.91	10	1
1:A:45:ILE:HG23	1:A:51:THR:CG2	0.42	2.39	15	2
1:A:130:VAL:O	1:A:130:VAL:HG22	0.42	2.15	19	1
1:B:59:ASP:O	1:B:62:ILE:HD11	0.42	2.14	20	1
1:A:52:TYR:C	1:A:74:VAL:HG12	0.42	2.40	2	5
1:B:105:VAL:HG12	1:B:119:ILE:HD13	0.42	1.90	3	1
1:A:56:ALA:CB	1:A:70:ASP:OD2	0.42	2.67	11	5
1:B:87:ILE:O	1:B:87:ILE:CG2	0.42	2.68	16	3
1:B:87:ILE:HD12	1:B:95:THR:O	0.42	2.14	6	1
1:A:85:ILE:CG2	1:B:139:ARG:C	0.42	2.93	7	1
1:A:101:LEU:CD1	1:A:101:LEU:C	0.42	2.93	7	1
1:B:40:LEU:HD12	1:B:40:LEU:O	0.42	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD13	1:B:43:LEU:HD12	0.42	1.90	14	1
1:A:59:ASP:O	1:A:62:ILE:CD1	0.42	2.68	20	2
1:A:44:LEU:HD12	1:B:71:LEU:HD12	0.42	1.90	17	1
1:B:59:ASP:O	1:B:62:ILE:CD1	0.42	2.67	20	1
1:A:56:ALA:CB	1:A:70:ASP:OD1	0.42	2.67	18	6
1:A:97:LYS:CD	1:A:108:ILE:O	0.42	2.68	6	2
1:A:137:ALA:CA	1:B:133:HIS:CD2	0.42	3.03	5	2
1:A:71:LEU:CD1	1:A:73:ILE:CD1	0.42	2.97	3	1
1:B:44:LEU:C	1:B:45:ILE:CG1	0.42	2.92	5	1
1:A:40:LEU:CD2	1:B:45:ILE:CD1	0.42	2.92	8	1
1:B:132:ILE:O	1:B:132:ILE:CG2	0.42	2.67	8	2
1:A:114:TYR:CD1	1:A:114:TYR:N	0.42	2.88	11	1
1:A:75:ASP:OD2	1:A:131:VAL:HG11	0.42	2.15	15	1
1:B:73:ILE:O	1:B:133:HIS:N	0.42	2.53	16	1
1:B:52:TYR:CB	1:B:74:VAL:O	0.42	2.68	17	1
1:B:84:ASP:O	1:B:86:VAL:HG13	0.42	2.13	20	1
1:A:64:GLY:O	1:A:134:VAL:CG1	0.42	2.67	1	1
1:A:86:VAL:HB	1:A:127:VAL:HG11	0.42	1.91	1	3
1:B:98:LYS:O	1:B:108:ILE:CG2	0.42	2.68	1	2
1:B:108:ILE:HD13	1:B:116:PRO:CA	0.42	2.44	2	1
1:B:43:LEU:CD1	1:B:44:LEU:HD13	0.42	2.44	5	1
1:A:99:LEU:HD22	1:A:127:VAL:HG22	0.42	1.90	7	1
1:A:130:VAL:HG13	1:A:131:VAL:N	0.42	2.30	7	1
1:B:130:VAL:HG13	1:B:131:VAL:N	0.42	2.30	7	1
1:B:52:TYR:O	1:B:74:VAL:O	0.42	2.38	12	1
1:A:78:ILE:HB	1:A:130:VAL:HG11	0.42	1.92	13	1
1:B:56:ALA:HB3	1:B:70:ASP:CG	0.42	2.40	17	1
1:A:139:ARG:O	1:B:132:ILE:HD13	0.42	2.15	19	1
1:A:63:ASP:CB	1:A:110:MET:HB2	0.42	2.45	1	1
1:B:55:LYS:CE	1:B:70:ASP:O	0.42	2.68	2	5
1:B:102:ARG:N	1:B:103:PRO:HD2	0.42	2.30	2	2
1:B:107:LEU:HD21	1:B:109:PRO:HG3	0.42	1.92	3	1
1:A:43:LEU:HD22	1:B:53:PHE:CE1	0.42	2.50	7	1
1:A:61:MET:O	1:A:66:ILE:CG1	0.42	2.67	7	1
1:A:139:ARG:C	1:B:85:ILE:CG2	0.42	2.93	7	1
1:A:137:ALA:HB2	1:B:133:HIS:CD2	0.42	2.50	8	1
1:A:99:LEU:HA	1:A:107:LEU:HD12	0.42	1.91	9	1
1:A:132:ILE:CG2	1:A:132:ILE:O	0.42	2.68	10	1
1:B:40:LEU:O	1:B:43:LEU:CD1	0.42	2.68	13	2
1:B:41:ASN:HB2	1:B:45:ILE:HD12	0.42	1.91	10	1
1:A:55:LYS:HG2	1:A:71:LEU:HD23	0.42	1.91	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:62:ILE:CD1	1:B:111:ASN:CG	0.42	2.93	12	2
1:A:40:LEU:CD2	1:B:41:ASN:HB2	0.42	2.45	13	1
1:B:45:ILE:CG2	1:B:46:GLN:N	0.42	2.82	13	1
1:B:45:ILE:HG23	1:B:51:THR:CG2	0.42	2.39	15	1
1:B:56:ALA:CB	1:B:70:ASP:CG	0.42	2.93	15	2
1:A:45:ILE:CG1	1:A:51:THR:HG21	0.42	2.44	19	1
1:B:88:ALA:HB2	1:B:99:LEU:HD13	0.42	1.91	19	1
1:A:130:VAL:O	1:A:130:VAL:CG2	0.42	2.67	3	4
1:A:44:LEU:HD22	1:A:44:LEU:N	0.42	2.30	4	1
1:A:63:ASP:OD1	1:A:96:VAL:O	0.42	2.38	11	4
1:B:56:ALA:CB	1:B:70:ASP:OD2	0.42	2.68	11	5
1:B:43:LEU:HG	1:B:44:LEU:N	0.42	2.29	6	1
1:A:96:VAL:O	1:A:97:LYS:CB	0.42	2.68	17	5
1:B:107:LEU:O	1:B:108:ILE:O	0.42	2.38	14	3
1:A:71:LEU:O	1:A:135:VAL:N	0.42	2.53	11	1
1:B:60:SER:O	1:B:111:ASN:N	0.42	2.53	20	2
1:B:74:VAL:O	1:B:74:VAL:CG1	0.42	2.68	17	1
1:B:86:VAL:HA	1:B:132:ILE:CD1	0.42	2.45	18	1
1:B:53:PHE:CD1	1:B:53:PHE:N	0.42	2.88	20	1
1:A:44:LEU:C	1:A:45:ILE:CG1	0.42	2.92	5	1
1:A:52:TYR:N	1:A:74:VAL:O	0.42	2.53	16	2
1:A:43:LEU:HD23	1:B:71:LEU:HD21	0.42	1.92	13	1
1:A:56:ALA:HB2	1:A:66:ILE:HG22	0.42	1.91	14	1
1:A:133:HIS:CD2	1:B:137:ALA:CA	0.41	3.03	5	2
1:B:52:TYR:C	1:B:74:VAL:HG12	0.41	2.40	6	7
1:A:51:THR:HG23	1:A:74:VAL:O	0.41	2.15	4	1
1:A:72:LEU:CD1	1:A:72:LEU:C	0.41	2.93	10	1
1:A:56:ALA:CB	1:A:70:ASP:CG	0.41	2.93	15	2
1:A:97:LYS:CG	1:A:108:ILE:O	0.41	2.68	18	1
1:A:55:LYS:CE	1:A:70:ASP:O	0.41	2.68	2	6
1:B:94:PHE:C	1:B:95:THR:HG23	0.41	2.39	1	1
1:A:43:LEU:HD21	1:B:71:LEU:CD1	0.41	2.37	3	1
1:B:63:ASP:OD1	1:B:96:VAL:O	0.41	2.38	3	4
1:B:61:MET:CB	1:B:66:ILE:HD11	0.41	2.45	4	1
1:A:99:LEU:CD2	1:A:127:VAL:CG2	0.41	2.96	7	1
1:A:59:ASP:OD1	1:A:59:ASP:N	0.41	2.53	8	4
1:A:95:THR:CG2	1:A:109:PRO:HG3	0.41	2.45	8	1
1:B:90:VAL:CG1	1:B:93:GLU:HB2	0.41	2.45	8	1
1:B:132:ILE:CG2	1:B:132:ILE:O	0.41	2.68	10	2
1:A:45:ILE:CG2	1:A:51:THR:OG1	0.41	2.69	18	2
1:A:40:LEU:HD12	1:A:40:LEU:O	0.41	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ILE:CD1	1:A:115:SER:C	0.41	2.93	15	1
1:A:52:TYR:CB	1:A:74:VAL:O	0.41	2.68	17	1
1:B:131:VAL:C	1:B:132:ILE:CD1	0.41	2.92	19	1
1:B:109:PRO:C	1:B:110:MET:HG2	0.41	2.39	3	1
1:B:44:LEU:HD22	1:B:44:LEU:H	0.41	1.75	4	1
1:B:95:THR:CG2	1:B:107:LEU:HD21	0.41	2.44	6	1
1:A:53:PHE:CE1	1:B:43:LEU:HD22	0.41	2.50	7	1
1:A:73:ILE:HD11	1:B:44:LEU:HD21	0.41	1.91	7	1
1:A:98:LYS:O	1:A:98:LYS:CG	0.41	2.68	8	2
1:B:101:LEU:C	1:B:101:LEU:CD1	0.41	2.92	9	1
1:A:71:LEU:C	1:A:72:LEU:HD23	0.41	2.40	11	1
1:B:78:ILE:HB	1:B:130:VAL:HG11	0.41	1.92	13	1
1:A:64:GLY:O	1:A:134:VAL:CG2	0.41	2.68	18	1
1:B:59:ASP:O	1:B:111:ASN:ND2	0.41	2.53	1	1
1:B:94:PHE:O	1:B:95:THR:CG2	0.41	2.68	1	1
1:A:41:ASN:OD1	1:A:42:GLN:N	0.41	2.54	2	4
1:A:43:LEU:CD1	1:A:43:LEU:C	0.41	2.86	11	1
1:B:71:LEU:C	1:B:72:LEU:HD23	0.41	2.41	11	1
1:A:52:TYR:O	1:A:74:VAL:O	0.41	2.38	12	1
1:B:39:ASP:OD1	1:B:41:ASN:ND2	0.41	2.53	17	2
1:B:95:THR:HB	1:B:108:ILE:HG21	0.41	1.91	13	1
1:A:73:ILE:O	1:A:133:HIS:N	0.41	2.53	16	2
1:B:64:GLY:O	1:B:134:VAL:CG2	0.41	2.67	18	1
1:A:131:VAL:C	1:A:132:ILE:CD1	0.41	2.92	19	1
1:A:96:VAL:HG13	1:A:131:VAL:HG13	0.41	1.91	20	1
1:A:39:ASP:OD2	1:A:43:LEU:N	0.41	2.53	2	1
1:A:40:LEU:HD11	1:B:41:ASN:HA	0.41	1.93	2	1
1:B:63:ASP:OD1	1:B:97:LYS:N	0.41	2.53	2	1
1:A:43:LEU:C	1:A:43:LEU:HD22	0.41	2.41	4	1
1:B:43:LEU:C	1:B:43:LEU:HD22	0.41	2.41	4	1
1:B:115:SER:CB	1:B:116:PRO:HD2	0.41	2.46	7	2
1:A:71:LEU:HD21	1:B:43:LEU:HD23	0.41	1.93	13	1
1:B:99:LEU:HD12	1:B:101:LEU:HD11	0.41	1.93	14	1
1:A:56:ALA:HB3	1:A:70:ASP:CG	0.41	2.40	17	1
1:A:39:ASP:OD1	1:A:41:ASN:ND2	0.41	2.53	1	2
1:A:67:SER:N	1:A:70:ASP:OD1	0.41	2.53	1	1
1:A:63:ASP:OD1	1:A:97:LYS:N	0.41	2.54	2	1
1:A:52:TYR:HB3	1:A:74:VAL:CG1	0.41	2.45	5	2
1:B:59:ASP:HA	1:B:62:ILE:CD1	0.41	2.46	5	1
1:B:59:ASP:OD1	1:B:59:ASP:N	0.41	2.54	17	2
1:A:78:ILE:CD1	1:A:130:VAL:HG11	0.41	2.43	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ALA:N	1:A:95:THR:O	0.41	2.54	15	2
1:B:63:ASP:OD2	1:B:108:ILE:CD1	0.41	2.66	16	1
1:A:44:LEU:CB	1:B:40:LEU:HD21	0.41	2.45	18	1
1:A:53:PHE:HB3	1:A:73:ILE:CD1	0.41	2.46	3	1
1:A:90:VAL:CG1	1:A:93:GLU:HB2	0.41	2.46	20	3
1:B:71:LEU:CD1	1:B:73:ILE:HD11	0.41	2.43	3	1
1:A:120:SER:CB	1:A:123:ASP:OD2	0.41	2.69	4	1
1:A:87:ILE:O	1:A:87:ILE:CG2	0.41	2.68	5	2
1:A:108:ILE:HD11	1:A:114:TYR:CA	0.41	2.46	6	1
1:A:43:LEU:HG	1:B:53:PHE:CD1	0.41	2.51	11	1
1:A:111:ASN:O	1:A:113:ALA:N	0.41	2.54	11	1
1:A:74:VAL:O	1:A:74:VAL:CG1	0.41	2.68	17	1
1:A:132:ILE:HD13	1:B:139:ARG:O	0.41	2.16	19	1
1:B:41:ASN:OD1	1:B:42:GLN:N	0.41	2.54	20	3
1:B:43:LEU:HB3	1:B:44:LEU:HD22	0.41	1.92	2	1
1:A:44:LEU:HD21	1:B:73:ILE:HD11	0.41	1.91	7	1
1:A:45:ILE:HG22	1:A:46:GLN:H	0.41	1.74	20	1
1:B:39:ASP:OD2	1:B:42:GLN:CB	0.41	2.69	1	1
1:B:56:ALA:CB	1:B:66:ILE:HA	0.41	2.46	2	4
1:A:56:ALA:CB	1:A:66:ILE:HA	0.41	2.45	5	3
1:A:95:THR:OG1	1:A:109:PRO:CB	0.41	2.69	2	1
1:B:108:ILE:CD1	1:B:115:SER:C	0.41	2.92	2	1
1:B:62:ILE:O	1:B:63:ASP:C	0.41	2.63	3	1
1:A:44:LEU:HD22	1:A:44:LEU:H	0.41	1.76	4	1
1:B:51:THR:HG23	1:B:74:VAL:O	0.41	2.15	4	1
1:B:52:TYR:N	1:B:74:VAL:O	0.41	2.54	5	1
1:A:134:VAL:HG12	1:B:136:LYS:O	0.41	2.15	7	1
1:A:95:THR:CG2	1:A:109:PRO:CG	0.41	2.98	8	1
1:A:100:GLN:OE1	1:A:103:PRO:CG	0.41	2.69	9	1
1:A:86:VAL:CG2	1:A:127:VAL:HG21	0.41	2.46	11	1
1:A:111:ASN:O	1:A:112:SER:C	0.41	2.63	11	1
1:B:55:LYS:HG2	1:B:71:LEU:HD23	0.41	1.91	11	1
1:A:41:ASN:HB2	1:B:40:LEU:CD2	0.41	2.45	13	1
1:A:82:HIS:CD2	1:A:102:ARG:CD	0.41	3.04	16	1
1:A:108:ILE:O	1:A:108:ILE:HG13	0.41	2.16	16	1
1:B:108:ILE:HD11	1:B:114:TYR:C	0.41	2.40	17	1
1:B:109:PRO:HG3	1:B:114:TYR:CZ	0.41	2.50	18	1
1:B:64:GLY:HA2	1:B:96:VAL:CG1	0.41	2.46	20	1
1:B:131:VAL:O	1:B:131:VAL:HG22	0.41	2.16	20	1
1:B:39:ASP:OD2	1:B:43:LEU:N	0.41	2.53	2	1
1:A:136:LYS:O	1:B:134:VAL:HG12	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:107:LEU:HB3	1:B:117:ILE:CG2	0.41	2.46	9	1
1:B:75:ASP:OD2	1:B:131:VAL:HG11	0.41	2.15	15	1
1:A:85:ILE:HG12	1:A:96:VAL:CG1	0.41	2.46	18	1
1:A:135:VAL:HG22	1:B:135:VAL:CG1	0.41	2.39	18	1
1:A:84:ASP:C	1:A:98:LYS:CG	0.40	2.94	4	1
1:B:61:MET:HE2	1:B:96:VAL:HG23	0.40	1.93	4	1
1:B:52:TYR:HB3	1:B:74:VAL:CG1	0.40	2.45	5	2
1:A:64:GLY:C	1:A:85:ILE:HD11	0.40	2.40	6	1
1:A:108:ILE:HD13	1:A:110:MET:N	0.40	2.31	7	1
1:A:133:HIS:CD2	1:B:137:ALA:HB2	0.40	2.50	8	1
1:A:119:ILE:CG2	1:A:120:SER:N	0.40	2.84	10	2
1:A:60:SER:O	1:A:61:MET:CG	0.40	2.69	14	1
1:B:117:ILE:O	1:B:117:ILE:CG2	0.40	2.67	14	1
1:A:47:HIS:CG	1:A:50:ALA:HB3	0.40	2.51	17	1
1:A:86:VAL:HA	1:A:132:ILE:CD1	0.40	2.45	18	1
1:A:38:ILE:O	1:A:38:ILE:CG1	0.40	2.69	19	1
1:A:65:GLY:CA	1:A:96:VAL:HG11	0.40	2.46	19	1
1:B:96:VAL:O	1:B:97:LYS:CG	0.40	2.69	1	1
1:A:47:HIS:ND1	1:A:75:ASP:OD1	0.40	2.54	3	1
1:A:59:ASP:HA	1:A:62:ILE:CD1	0.40	2.46	4	2
1:A:40:LEU:HD21	1:B:41:ASN:HA	0.40	1.93	13	1
1:A:40:LEU:HA	1:A:43:LEU:CB	0.40	2.46	14	1
1:A:63:ASP:CG	1:A:96:VAL:O	0.40	2.64	20	2
1:A:41:ASN:HA	1:B:40:LEU:HD11	0.40	1.92	2	1
1:B:44:LEU:HD22	1:B:44:LEU:N	0.40	2.30	4	1
1:A:54:VAL:HG13	1:A:54:VAL:O	0.40	2.16	7	1
1:A:40:LEU:HG	1:B:45:ILE:CD1	0.40	2.47	10	1
1:B:41:ASN:O	1:B:45:ILE:HB	0.40	2.17	10	1
1:B:108:ILE:O	1:B:108:ILE:HG13	0.40	2.16	10	1
1:B:97:LYS:HB2	1:B:108:ILE:CB	0.40	2.47	11	1
1:A:110:MET:O	1:A:111:ASN:C	0.40	2.63	14	1
1:A:93:GLU:O	1:A:94:PHE:CG	0.40	2.74	18	1
1:A:96:VAL:HG13	1:A:131:VAL:CG1	0.40	2.46	20	1
1:A:130:VAL:CG1	1:B:139:ARG:HA	0.40	2.46	20	1
1:A:131:VAL:O	1:A:131:VAL:HG22	0.40	2.16	20	1
1:A:62:ILE:O	1:A:63:ASP:C	0.40	2.63	3	1
1:A:39:ASP:OD2	1:A:42:GLN:CB	0.40	2.69	4	1
1:B:43:LEU:N	1:B:43:LEU:CD1	0.40	2.84	10	1
1:A:53:PHE:CD1	1:B:43:LEU:HG	0.40	2.51	11	1
1:A:85:ILE:CD1	1:B:138:MET:HG2	0.40	2.46	14	1
1:B:107:LEU:O	1:B:117:ILE:HG22	0.40	2.16	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:HIS:CG	1:B:50:ALA:HB3	0.40	2.50	17	1
1:B:130:VAL:O	1:B:130:VAL:HG22	0.40	2.15	19	1
1:A:139:ARG:HA	1:B:130:VAL:CG1	0.40	2.46	20	1
1:A:76:SER:HB2	1:A:128:PHE:CD2	0.40	2.52	1	1
1:B:53:PHE:HB3	1:B:73:ILE:CD1	0.40	2.46	3	1
1:A:64:GLY:HA3	1:A:96:VAL:CG1	0.40	2.47	6	1
1:B:54:VAL:O	1:B:54:VAL:HG13	0.40	2.16	7	1
1:A:43:LEU:HD11	1:B:73:ILE:HD12	0.40	1.92	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/115 (88%)	70±3 (69±3%)	21±3 (21±3%)	10±2 (10±2%)	1	10
1	B	101/115 (88%)	70±3 (69±3%)	21±3 (21±3%)	10±3 (10±3%)	1	9
All	All	4040/4600 (88%)	2792 (69%)	849 (21%)	399 (10%)	1	10

All 61 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	77	ALA	20
1	B	77	ALA	20
1	A	80	ALA	13
1	B	80	ALA	13
1	A	68	ASP	13
1	B	68	ASP	13
1	B	120	SER	13
1	A	120	SER	12
1	B	132	ILE	11
1	A	85	ILE	11
1	B	85	ILE	11
1	A	59	ASP	10
1	A	132	ILE	10

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Mol	Chain	Res	Type	Models (Total)
1	A	109	PRO	10
1	B	109	PRO	10
1	A	46	GLN	9
1	B	46	GLN	9
1	B	59	ASP	9
1	A	38	ILE	9
1	A	123	ASP	9
1	B	123	ASP	9
1	A	130	VAL	8
1	B	130	VAL	8
1	B	38	ILE	8
1	A	45	ILE	8
1	B	45	ILE	8
1	B	111	ASN	8
1	A	69	GLY	7
1	B	69	GLY	7
1	A	121	SER	6
1	B	65	GLY	6
1	B	110	MET	5
1	A	65	GLY	5
1	A	111	ASN	5
1	B	108	ILE	5
1	B	121	SER	5
1	A	49	SER	4
1	B	49	SER	4
1	B	96	VAL	4
1	B	112	SER	3
1	A	40	LEU	3
1	A	96	VAL	3
1	B	40	LEU	3
1	A	64	GLY	3
1	B	64	GLY	3
1	B	113	ALA	3
1	A	112	SER	2
1	A	108	ILE	2
1	B	115	SER	2
1	B	97	LYS	2
1	A	61	MET	2
1	A	119	ILE	2
1	B	61	MET	2
1	A	97	LYS	2
1	A	110	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	113	ALA	1
1	A	50	ALA	1
1	B	50	ALA	1
1	A	48	PRO	1
1	B	48	PRO	1
1	B	119	ILE	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/97 (90%)	68±3 (78±3%)	19±3 (22±3%)	3	30
1	B	87/97 (90%)	68±2 (78±3%)	19±2 (22±3%)	3	30
All	All	3480/3880 (90%)	2726 (78%)	754 (22%)	3	30

All 103 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	43	LEU	20
1	A	55	LYS	20
1	B	43	LEU	20
1	B	55	LYS	20
1	A	87	ILE	18
1	B	87	ILE	18
1	A	102	ARG	16
1	B	102	ARG	16
1	B	108	ILE	16
1	A	44	LEU	15
1	A	97	LYS	15
1	A	108	ILE	15
1	A	125	LEU	15
1	B	44	LEU	15
1	B	125	LEU	15
1	A	40	LEU	14
1	B	40	LEU	14
1	B	98	LYS	14

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Mol	Chain	Res	Type	Models (Total)
1	A	52	TYR	13
1	A	132	ILE	13
1	B	52	TYR	13
1	B	97	LYS	13
1	B	132	ILE	13
1	A	61	MET	13
1	B	61	MET	13
1	A	110	MET	11
1	B	110	MET	11
1	A	98	LYS	10
1	A	46	GLN	9
1	B	38	ILE	9
1	B	46	GLN	9
1	B	136	LYS	9
1	A	138	MET	9
1	B	138	MET	9
1	A	139	ARG	9
1	B	139	ARG	9
1	A	107	LEU	8
1	A	136	LYS	8
1	A	38	ILE	8
1	A	117	ILE	8
1	A	123	ASP	8
1	B	123	ASP	8
1	A	121	SER	7
1	B	121	SER	7
1	B	96	VAL	7
1	B	122	GLU	7
1	B	117	ILE	7
1	A	120	SER	6
1	B	120	SER	6
1	A	71	LEU	6
1	A	96	VAL	6
1	B	71	LEU	6
1	B	100	GLN	6
1	A	93	GLU	6
1	A	42	GLN	6
1	B	42	GLN	6
1	A	100	GLN	6
1	A	122	GLU	6
1	A	67	SER	5
1	A	85	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	B	85	ILE	5
1	A	49	SER	4
1	A	128	PHE	4
1	B	49	SER	4
1	B	128	PHE	4
1	A	57	SER	4
1	B	57	SER	4
1	B	67	SER	4
1	B	93	GLU	4
1	B	95	THR	4
1	A	104	THR	4
1	A	66	ILE	4
1	B	66	ILE	4
1	A	72	LEU	3
1	B	72	LEU	3
1	B	104	THR	3
1	A	95	THR	3
1	B	94	PHE	3
1	A	94	PHE	2
1	A	106	GLN	2
1	B	106	GLN	2
1	A	111	ASN	2
1	B	115	SER	2
1	A	68	ASP	2
1	B	68	ASP	2
1	A	60	SER	2
1	B	60	SER	2
1	A	131	VAL	2
1	B	131	VAL	2
1	B	107	LEU	1
1	B	111	ASN	1
1	A	133	HIS	1
1	B	133	HIS	1
1	B	91	ASP	1
1	B	105	VAL	1
1	A	115	SER	1
1	A	91	ASP	1
1	A	47	HIS	1
1	B	47	HIS	1
1	A	45	ILE	1
1	A	75	ASP	1
1	B	45	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	75	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided